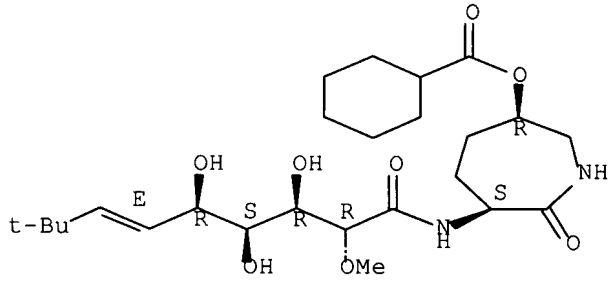
L10 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1295643 CAPLUS Full-text
DN 146:134828
TI A phase I and pharmacokinetic study of LAF389 administered to patients with advanced cancer
AU Dumez, Herlinde; Gall, Helen; Capdeville, Renaud; Dutreix, Catherine; van Oosterom, Allan T.; Giaccone, Giuseppe
CS KUL UZ Gasthuisberg, Louvain, Belg.
SO Anti-Cancer Drugs (2007), 18(2), 219-225
CODEN: ANTDEV; ISSN: 0959-4973
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB LAF389 is a synthetic analog of bengamide B, a natural product isolated from Jaspidae sponges. LAF389 has both antiproliferative and antiangiogenetic properties, and preclin. investigations showed a broad antitumor activity. This clin. trial aimed to determine the safety and pharmacokinetic profile of LAF389 administered as a slow i.v. injection for 3 consecutive days every 3 wk in patients with advanced solid tumors. Eight dose levels were tested: 1, 2.5, 5, 10, 15, 30, 25 and 20 mg/day. A total of 33 patients, median age 52 years (range 33-72), with refractory solid tumors were enrolled, 19 men and 14 women with a median World Health Organization performance status of 1 (0-4). Seventy-eight cycles of treatment have been administered (mean 2.5, range 1-10). Four cardiovascular dose-limiting toxicities were reported at 30 mg (2/2 patients) and 25 mg (2/9 patients), eight addnl. patients at various dose levels had (cardio)vascular toxicity, probably drug related, and one patient died owing to pulmonary embolism at the 5 mg dose. No objective responses were recorded. Pharmacokinetic parameters were variable, although linear and without obvious accumulation from cycle I to cycle II. LAF389 dose escalation was terminated owing to occurrence of unpredictable cardiovascular events. This, associated with the lack of clin. activity, did not warrant further investigation of this agent.
IT 270902-51-7, LAF389
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phase I and pharmacokinetic study of LAF389)
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

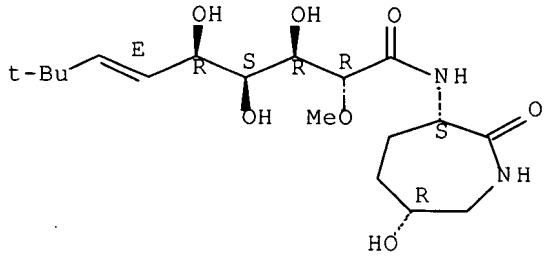
Absolute stereochemistry.
Double bond geometry as shown.



IT 661482-39-9, LAF 153
RL: PKT (Pharmacokinetics); BIOL (Biological study)
(phase I and pharmacokinetic study of LAF389)
RN 661482-39-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-

2-oxo-1H-azepin-3-yl]-8,8-dimethyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1094948 CAPLUS Full-text
DN 145:417036
TI Chimeric anti-CD25 antibodies in immunotherapy of proliferative or infectious diseases
IN Katopodis, Andreas
PA Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SO PCT Int. Appl., 23pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006108670	A2	20061019	WO 2006-EP3444	20060413
WO 2006108670	A3	20061228		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

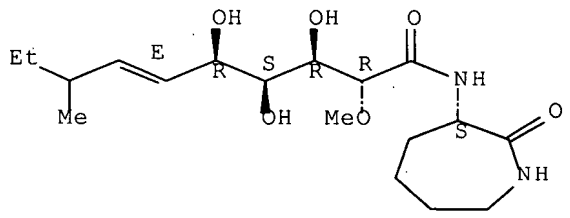
PRAI GB 2005-7696 A 20050415

AB A method is disclosed for the treatment of proliferative disease or infectious disease, where the inhibition of regulatory T cells is beneficial, that comprises administering to the patient an effective amount of an anti-CD25 antibody. The example describes the use of anti-CD25 antibody (basiliximab) in the maintenance of remission of colorectal cancer. In the clin. trial the patients are randomized to receive either standard cancer treatment or the standard treatment plus 1-10 mg/kg of basiliximab every two weeks.

IT 851794-49-5, Bengamide
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chimeric anti-CD25 antibodies in immunotherapy of proliferative or infectious diseases in combination with)

RN 851794-49-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



L10 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:511027 CAPLUS Full-text
DN 145:28210
TI Preparation of 2-alkoxy-3,4,5-trihydroxy-alkylamides with a substituted lactam ring, analogs of bengamide E, and their compositions containing them for treating antiproliferative diseases, particularly cancer
IN Zhang, Jidong; Bhatnagar, Neerja; Ruxer, Jean-Marie
PA Aventis Pharma S.A., Fr.
SO PCT Int. Appl., 89 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006056696	A2	20060601	WO 2005-FR2932	20051125
	WO 2006056696	A3	20060831		
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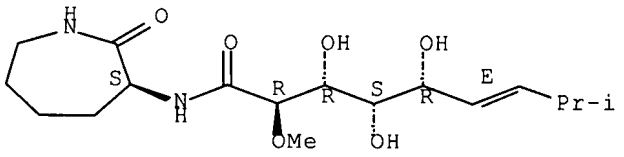
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	FR 2878528	A1	20060602	FR 2004-12645	20041129
PRAI	FR 2004-12645	A	20041129		

OS MARPAT 145:28210
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = CH:C(R11)(R12), CH:N-O(R4), CH:N(R4), hetero/aryl, etc.; R11, R12 = independently H, alkyl; R4 = H, alkyl, alkylaryl, alkylheteroaryl; X = (CH2)n; n = 1-4; R3 = alkyl, alkyl/alkylhetero/aryl, etc.; R = H, alkyl, benzyl, etc.] were prepared as antiproliferative, especially, antitumor agents. Thus, reacting lactone II with (7S,12bR)-7-amino- 1,34,7,8,12b-hexahydropyrido[2,1-a][2]benzazepin-6(2H)-one, followed by 1,3-acetonide deprotection gave title compound III. I displayed antiproliferative activity against Hep-G2 or HCT116 cell lines. Pharmaceutical compns. containing polyhydroxylated compds. I are claimed.
IT 118477-03-5P, Bengamide E
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(analogs; antiproliferative agents; preparation of 2-alkoxy-3,4,5-trihydroxy-alkylamides with a substituted lactam ring, analogs of bengamide E, for treating antiproliferative diseases, particularly cancer)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

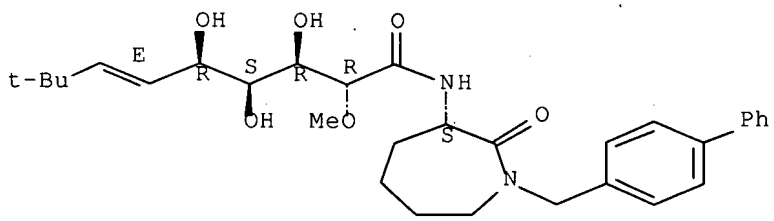
Absolute stereochemistry.
Double bond geometry as shown.



IT 889214-12-4P 889214-14-6P 889214-15-7P
889214-16-8P 889214-17-9P 889214-20-4P
889214-32-8P 889214-33-9P 889214-88-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiproliferative agent; preparation of 2-alkoxy-3,4,5-trihydroxy-alkylamides with a substituted lactam ring, analogs of bengamide E, for treating antiproliferative diseases, particularly cancer)

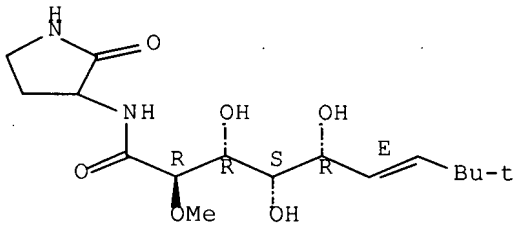
RN 889214-12-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-([1,1'-biphenyl]-4-ylmethyl)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



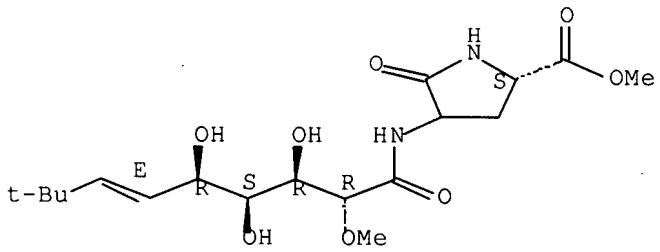
RN 889214-14-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-N-(2-oxo-3-pyrrolidinyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



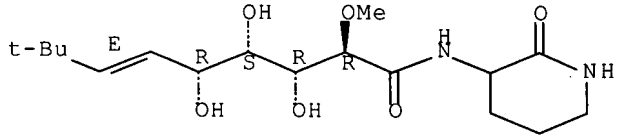
RN 889214-15-7 CAPLUS
CN L-Proline, 5-oxo-4-[[(6E)-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



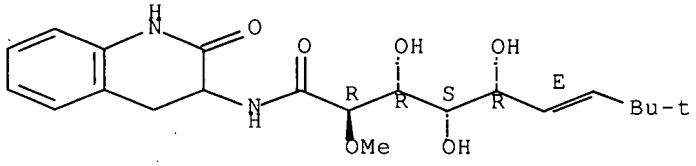
RN 889214-16-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-N-(2-oxo-3-piperidinyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



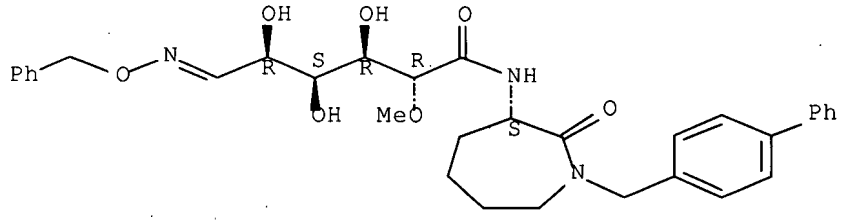
RN 889214-17-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-N-(1,2,3,4-tetrahydro-2-oxo-3-quinolinyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



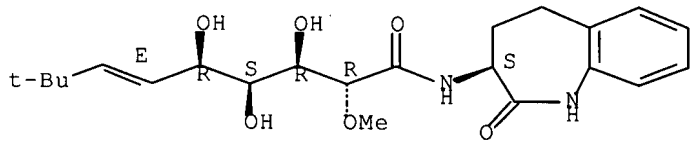
RN 889214-20-4 CAPLUS
CN L-Glucuronamide, N-[(3S)-1-([1,1'-biphenyl]-4-ylmethyl)hexahydro-2-oxo-1H-azepin-3-yl]-5-O-methyl-, 1-[O-(phenylmethyl)oxime] (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



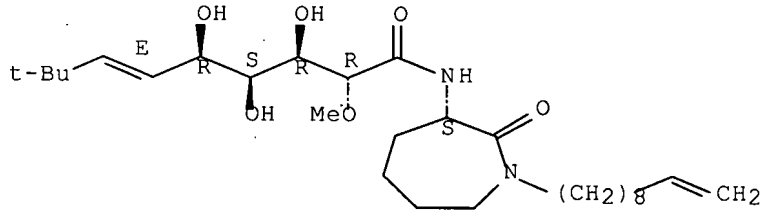
RN 889214-32-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-N-[(3S)-2,3,4,5-tetrahydro-2-oxo-1H-1-benzazepin-3-yl]-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



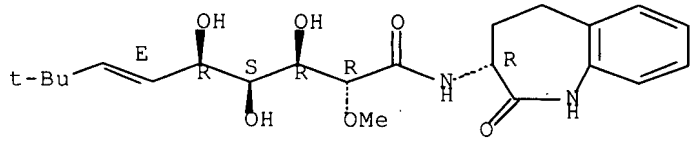
RN 889214-33-9 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-(9-decenyl)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



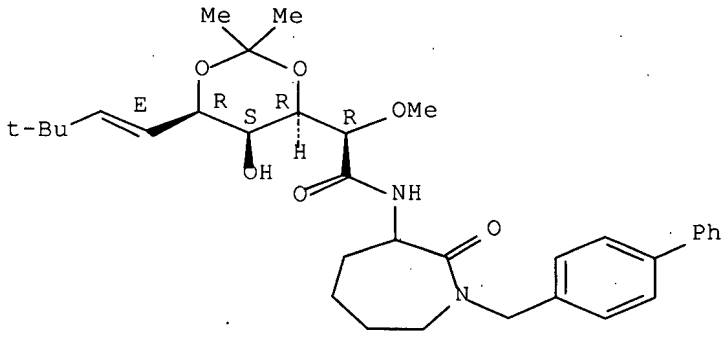
RN 889214-88-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-N-[(3R)-2,3,4,5-tetrahydro-2-oxo-1H-1-benzazepin-3-yl]-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



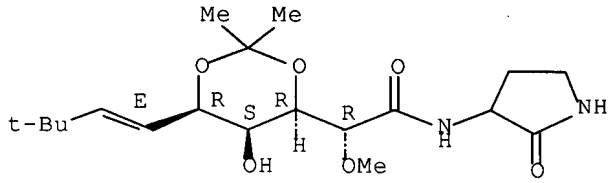
IT 889214-38-4P 889214-40-8P 889214-41-9P
889214-42-0P 889214-43-1P 889214-48-6P
889214-79-3P 889214-80-6P 889214-83-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 2-alkoxy-3,4,5-trihydroxy-alkylamides with a substituted lactam ring, analogs of bengamide E, for treating antiproliferative diseases, particularly cancer)
RN 889214-38-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[1-([1,1'-biphenyl]-4-ylmethyl)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



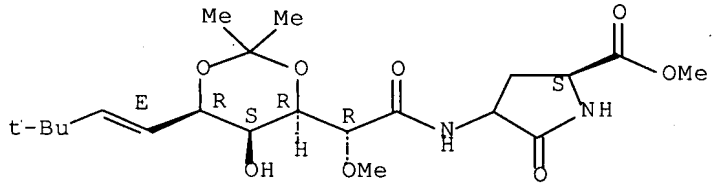
RN 889214-40-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-N-(2-oxo-3-pyrrolidinyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



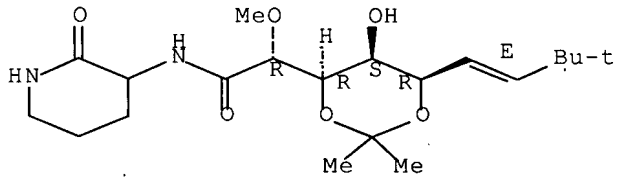
RN 889214-41-9 CAPLUS
CN L-Proline, 5-oxo-4-[[(6E)-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-D-gulo-non-6-enonoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



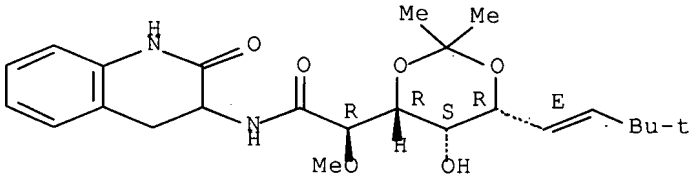
RN 889214-42-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-N-(2-oxo-3-piperidinyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



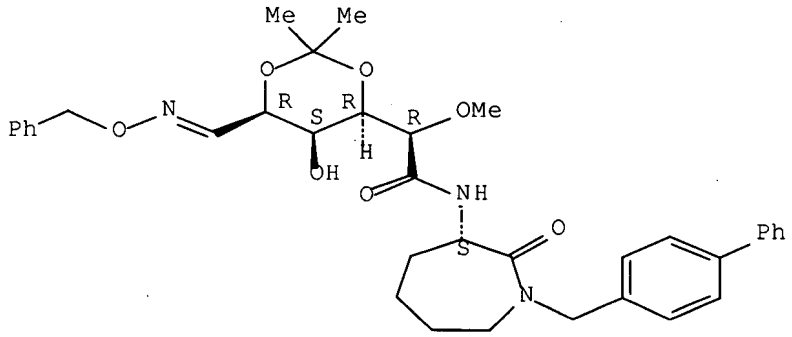
RN 889214-43-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-N-(1,2,3,4-tetrahydro-2-oxo-3-quinolinyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



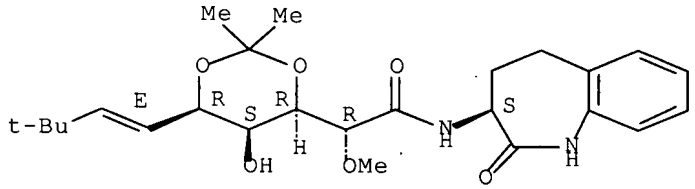
RN 889214-48-6 CAPLUS
CN L-Glucuronamide, N-[(3S)-1-([1,1'-biphenyl]-4-ylmethyl)hexahydro-2-oxo-1H-azepin-3-yl]-5-O-methyl-2,4-O-(1-methylethylidene)-, 1-[O-(phenylmethyl)oxime] (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



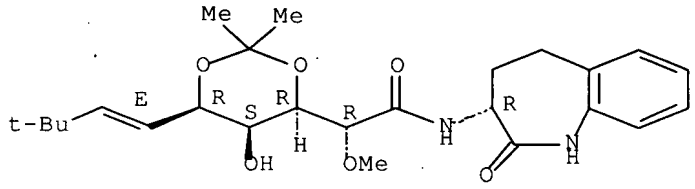
RN 889214-79-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-N-[(3S)-2,3,4,5-tetrahydro-2-oxo-1H-1-benzazepin-3-yl]-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 889214-80-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-N-[(3R)-2,3,4,5-tetrahydro-2-oxo-1H-1-benzazepin-3-yl]-, (6E)- (9CI) (CA INDEX NAME)

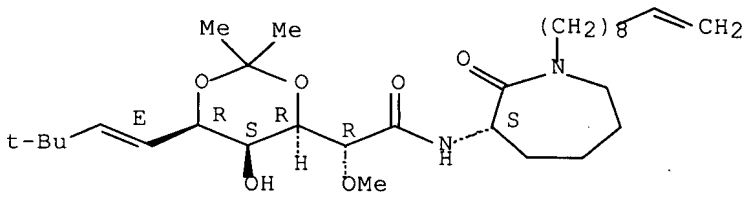
Absolute stereochemistry.
Double bond geometry as shown.



RN 889214-83-9 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S)-1-(9-decenyl)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:510431 CAPLUS Full-text
DN 145:27765
TI Method for the preparation of bengamides with a substituted caprolactam ring and compositions containing them for use as antiproliferative agents
IN Zhang, Jidong; Bhatnagar, Neerja
PA Aventis Pharma S.A., Fr.
SO PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006056695	A1	20060601	WO 2005-FR2931	20051125
	WO 2006056695	A8	20070405		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
	FR 2878525	A1	20060602	FR 2004-12646	20041129
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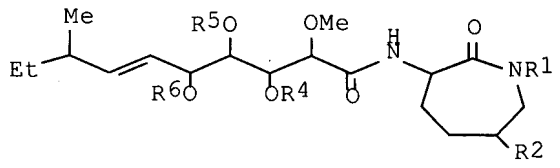
PRAI	FR 2004-12646	A	20041129		

OS CASREACT 145:27765; MARPAT 145:27765
GI



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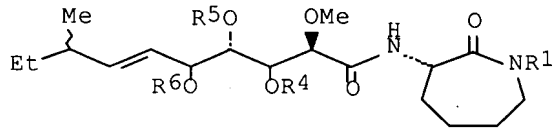


II

AB Method for the preparation of substituted caprolactams I [R1 = H, C1-24-alkyl, C3-9-cycloalkyl, heterocyclyl, C3-24-alkylene, heterocyclylalkylene, aryl, heteroaryl, arylalkly, hetteroarylalkyl, arylalkylene, heteroarylalkylene, (C1-8-alkyl)aryl(C1-24-alkyl), (C1-8-alkyl)aryl-O-(C1-24-alkyl); R2 = H, OR7, OC(:O)R7; R4, R5, R6 = H, C1-6-acyl, C1-6-alkyl, (C1-6-alkyl)aryl, (C1-6-alkyl)heteroaryl, aryl, heteroaryl, arylalkylene, heteroarylalkylene; R7 = C1-24-alkyl, C3-9-cycloalkyl, heterocyclyl, C3-24-alkylene, heterocyclylalkylene, aryl, heteroaryl, arylalkly, hetteroarylalkyl, arylalkylene, heteroarylalkylene, (C1-8-alkyl)aryl(C1-24- alkyl), (C1-8-alkyl)aryl-O-(C1-24-alkyl)] , compns. containing them and use thereof are described. Thus, bengamide II [R1 = R2 = R4 = R5 = R6 = H] was isolated from Myxococcus virescens, acetylated to give triacetate II [R1 = R2 = H, R4 = R5 = R6 = Ac] and alkylated with benzyl bromide to give II [R1 = CH2Ph, R2 = H, R4 = R5 = R6 = Ac] and then deacetylated to give II [R1 = CH2Ph, R2 = R4 = R5 = R6 = H].

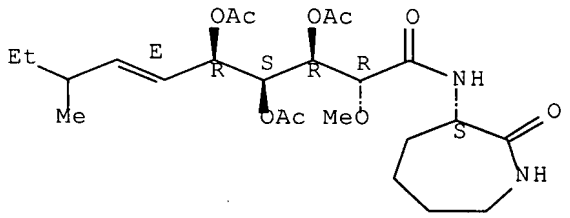
The invention relates to the preparation of substituted caprolactames, a method for the preparation thereof, compns. containing them and the use thereof as a medicament, particularly as anticancer agents. The antiproliferative activity of II [R1 = CH2Ph, R2 = R4 = R5 = R6 = H] was determined [IC50 = 0.02 μM vs. HEP-G2 cells].

IT 888481-88-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)(preparation and N-alkylation of, with benzyl halides; preparation of bengamides with a substituted caprolactam ring and compns. containing them for use as antiproliferative agents)

RN 888481-88-7 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

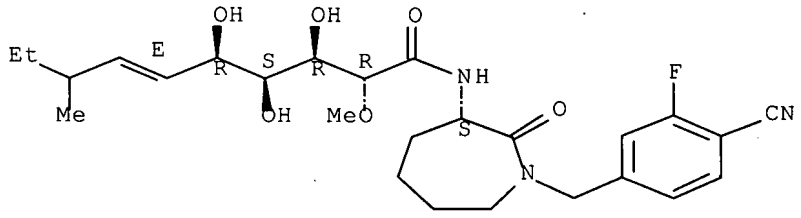


IT 888482-10-8P 888482-12-0P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and cyclization of, with hydrazine; preparation of bengamides with a substituted caprolactam ring and compns. containing them for use as antiproliferative agents)

RN 888482-10-8 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S)-1-[(4-cyano-3-fluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

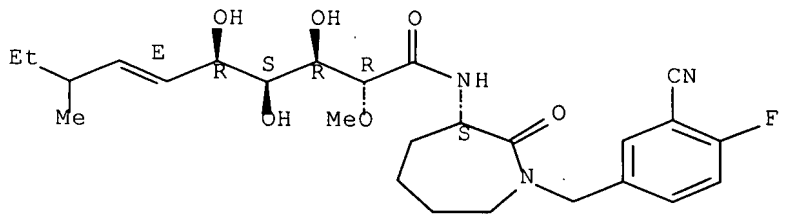
Absolute stereochemistry.
Double bond geometry as shown.



RN 888482-12-0 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S)-1-[(3-cyano-4-fluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

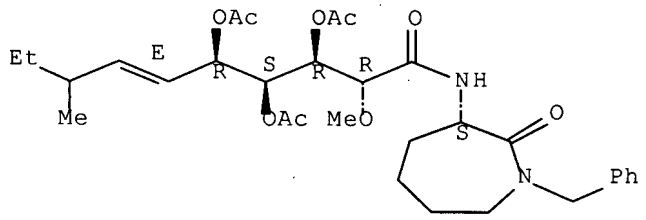
Absolute stereochemistry.
Double bond geometry as shown.



IT 888481-89-8P 888481-91-2P 888481-93-4P
888481-95-6P 888481-97-8P 888481-99-0P
888482-01-7P 888482-03-9P 888482-05-1P
888482-07-3P 888482-09-5P 888482-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of; preparation of bengamides with a substituted
caprolactam ring and compns. containing them for use as antiproliferative agents)

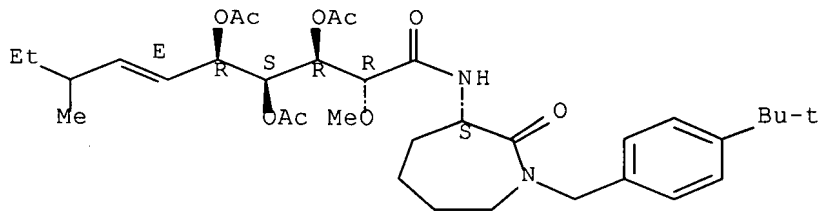
RN 888481-89-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-(phenylmethyl)-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



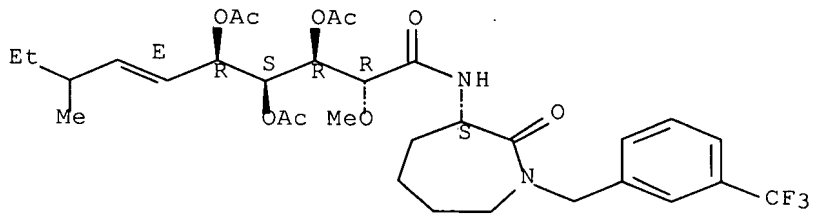
RN 888481-91-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-1-[[4-(1,1-dimethylethyl)phenyl]methyl]hexahydro-2-oxo-1H-azepin-3-yl]-8-ethyl-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



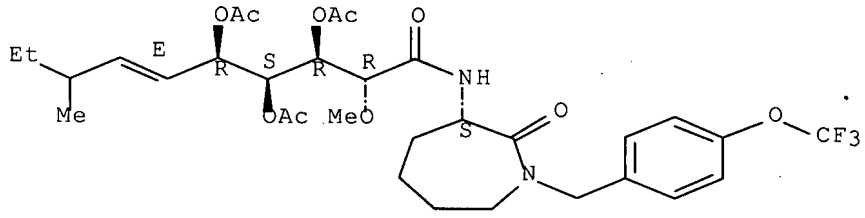
RN 888481-93-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[[3-(trifluoromethyl)phenyl]methyl]-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



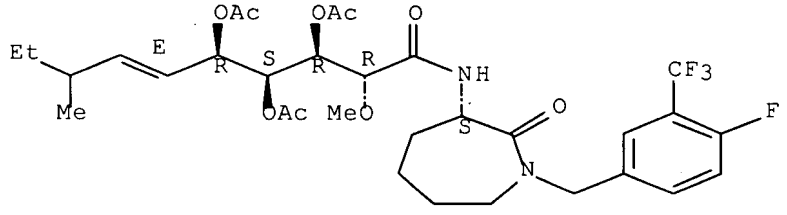
RN 888481-95-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[[4-(trifluoromethoxy)phenyl]methyl]-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



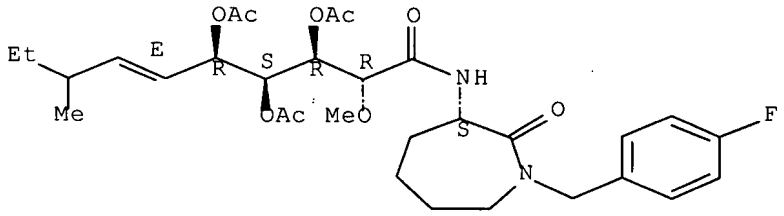
RN 888481-97-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-1-[[4-fluoro-3-(trifluoromethyl)phenyl]methyl]hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



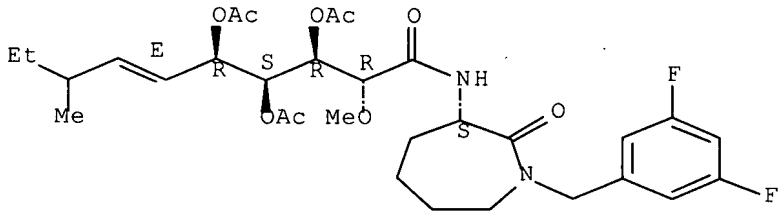
RN 888481-99-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-1-[(4-fluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



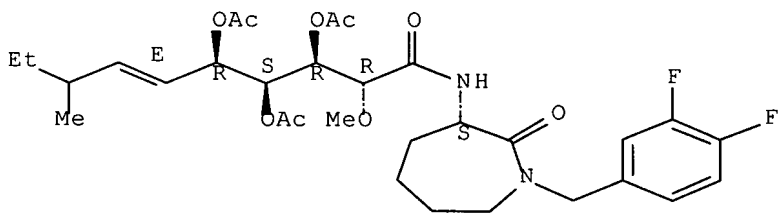
RN 888482-01-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-1-[(3,5-difluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-8-ethyl-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 888482-03-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-1-[(3,4-difluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-8-ethyl-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

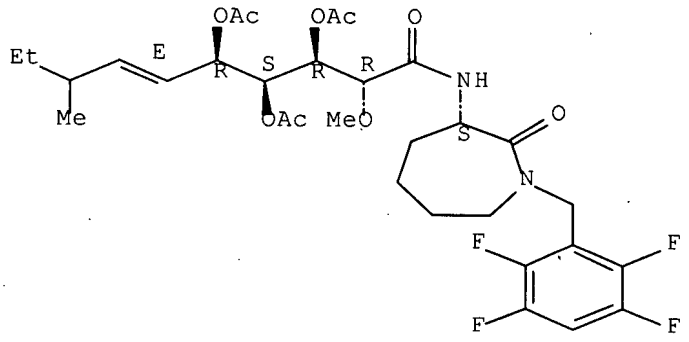
Absolute stereochemistry.
Double bond geometry as shown.



RN 888482-05-1 CAPLUS

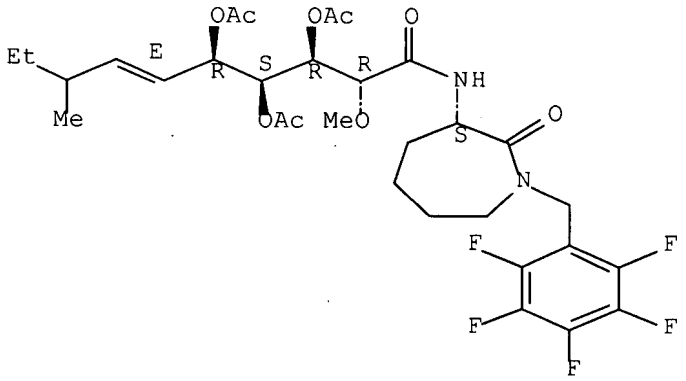
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[(2,3,5,6-tetrafluorophenyl)methyl]-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



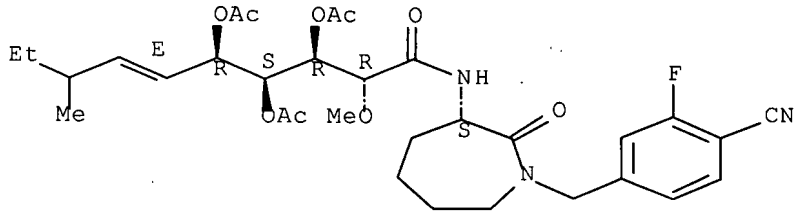
RN 888482-07-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[(pentafluorophenyl)methyl]-1H-azepin-3-yl]-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



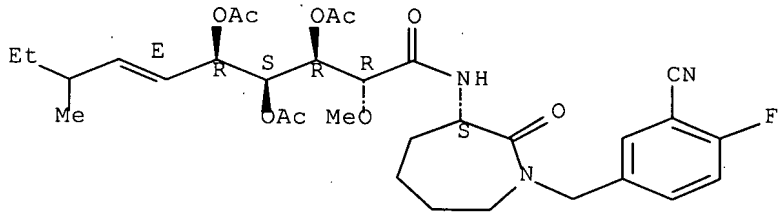
RN 888482-09-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-[(4-cyano-3-fluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-ethyl-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



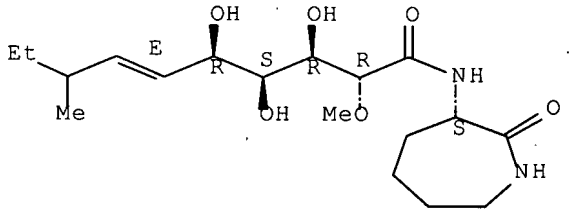
RN 888482-11-9 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-[(3-cyano-4-fluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-ethyl-2-O-methyl-, 3,4,5-triacetate, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 851794-49-5D, Bengamide, natural
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); RACT (Reactant or reagent); USES (Uses)
(preparation of bengamides with a substituted caprolactam ring and compns. containing them for use as antiproliferative agents)
RN 851794-49-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.

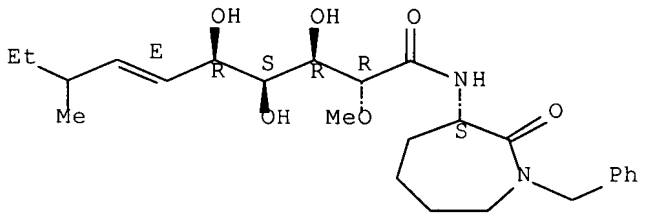


IT 888481-90-1P 888481-92-3P 888481-94-5P
888481-96-7P 888481-98-9P 888482-00-6P
888482-02-8P 888482-04-0P 888482-06-2P

888482-08-4P 888482-13-1P 888482-14-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bengamides with a substituted caprolactam ring and compns. containing them for use as antiproliferative agents)

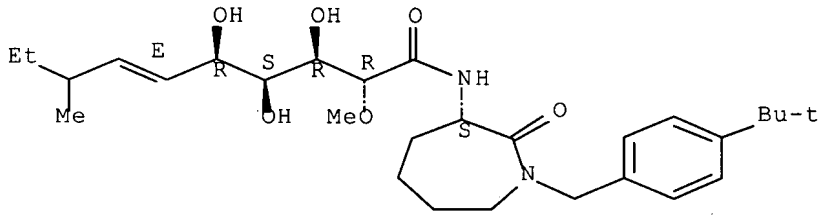
RN 888481-90-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-(phenylmethyl)-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



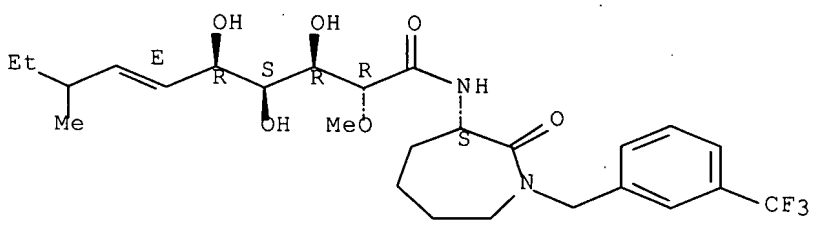
RN 888481-92-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-1-[[4-(1,1-dimethylethyl)phenyl]methyl]hexahydro-2-oxo-1H-azepin-3-yl]-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



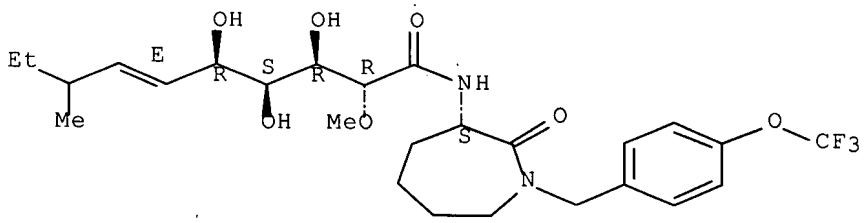
RN 888481-94-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[[3-(trifluoromethyl)phenyl]methyl]-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



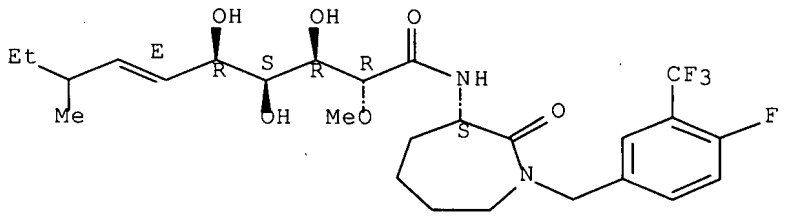
RN 888481-96-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[[4-(trifluoromethoxy)phenyl]methyl]-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



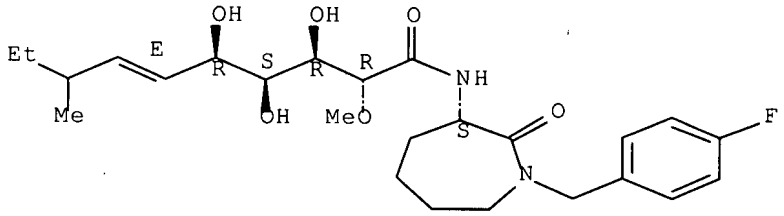
RN 888481-98-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-1-[[4-fluoro-3-(trifluoromethyl)phenyl]methyl]hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



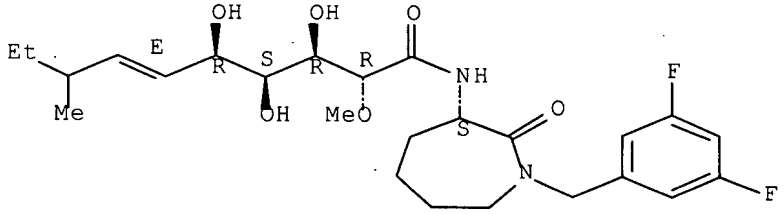
RN 888482-00-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-1-[(4-fluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



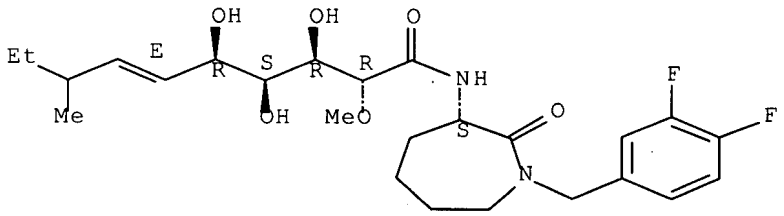
RN 888482-02-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-1-[(3,5-difluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



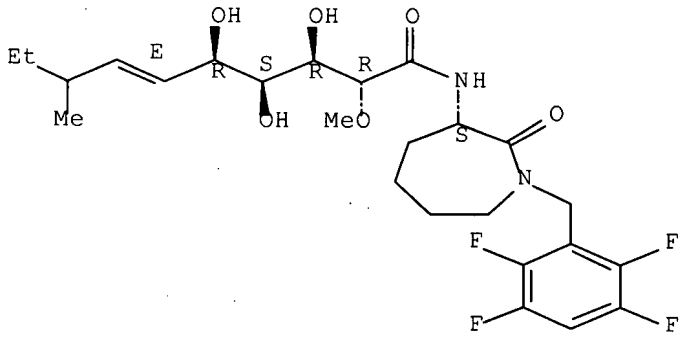
RN 888482-04-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-1-[(3,4-difluorophenyl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



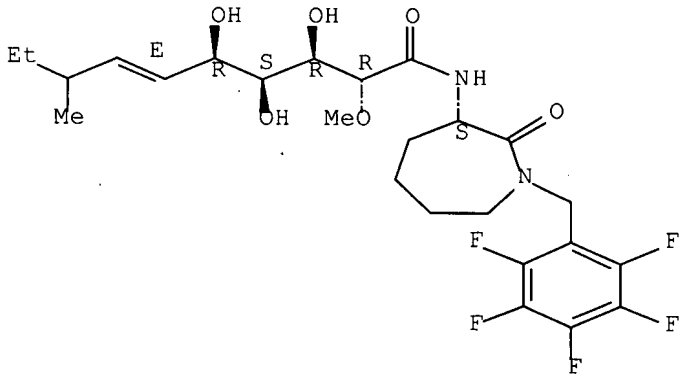
RN 888482-06-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[(2,3,5,6-tetrafluorophenyl)methyl]-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



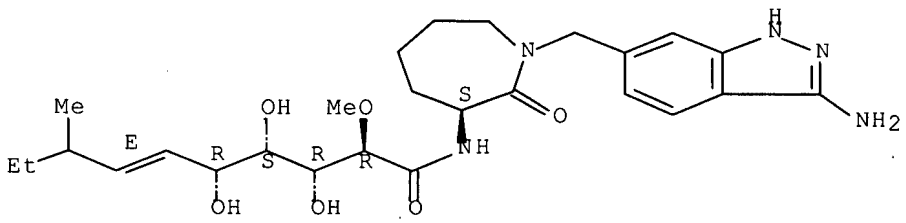
RN 888482-08-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1-[(pentafluorophenyl)methyl]-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



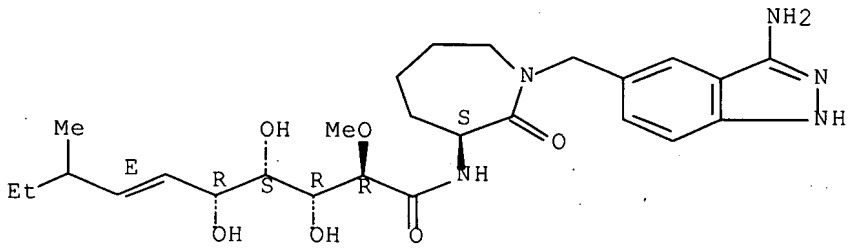
RN 888482-13-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-[(3-amino-1H-indazol-6-yl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 888482-14-2 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-[(3-amino-1H-indazol-5-yl)methyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-ethyl-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

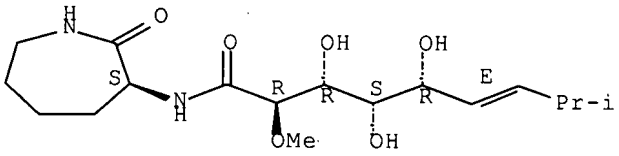
Absolute stereochemistry.
Double bond geometry as shown.



IT 118477-03-5, Bengamide E 851794-52-0 851794-54-2
888482-15-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of bengamides with a substituted caprolactam ring and compns. containing them for use as antiproliferative agents)

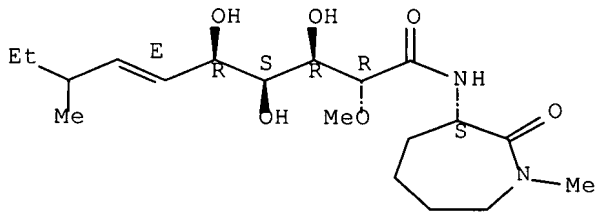
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



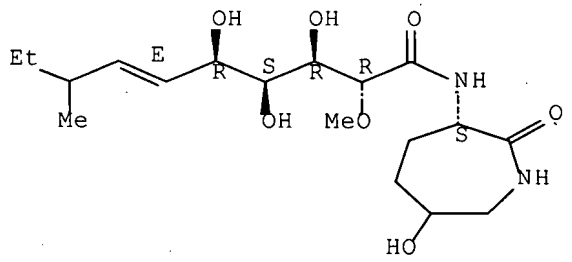
RN 851794-52-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



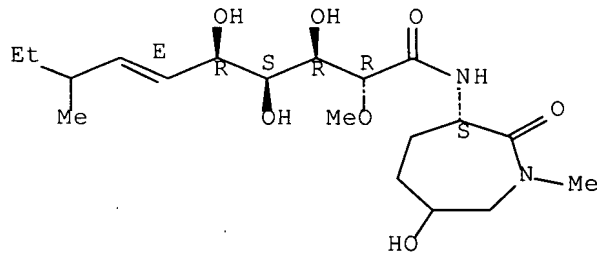
RN 851794-54-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



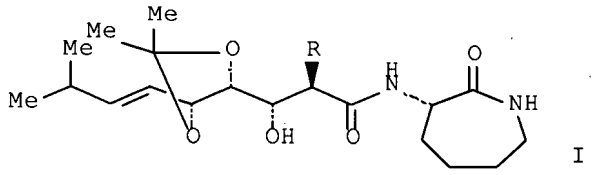
RN 888482-15-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

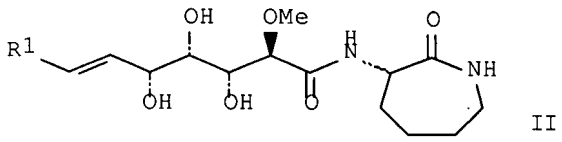


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1080544 CAPLUS Full-text
DN 144:23097
TI Total Synthesis of Bengamide E and Analogues by Modification at C-2 and at Terminal Olefinic Positions
AU Sarabia, Francisco; Sanchez-Ruiz, Antonio
CS Department of Biochemistry Molecular Biology and Organic Chemistry, Faculty of Sciences University of Malaga, Malaga, 29071, Spain
SO Journal of Organic Chemistry (2005), 70(23), 9514-9520
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 144:23097
GI



I



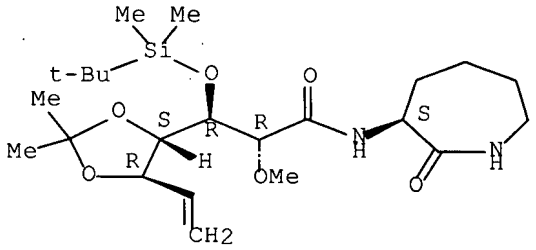
II

AB The total synthesis of the natural product bengamide E, one of the members of a new class of antitumor natural products of marine origin, is reported based on a convergent and flexible synthetic route featuring an oxirane ring-opening reaction and an olefin cross metathesis. In a similar way, bengamide analogs I (R = NH2, NHMe, NMe2, Cl) and II (R1 = CMe3, Ph; bengamide E has R1 = CHMe2), structurally modified at C-2 and at the terminal vinyl positions, resp., were prepared by introduction of various nucleophiles and alkyl substituents during the epoxide opening and the olefin cross metathesis steps, resp. These studies demonstrate the validity of this synthetic strategy, although they reveal some problems associated with the olefin cross metathesis, whose efficiency depends on the substituent at the C-2 position as well as the steric environment of the alkene.

IT 870093-45-1P 870093-46-2P 870093-48-4P
870093-49-5P 870093-50-8P 870093-67-7P
870093-68-8P 870093-69-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of bengamide E and its analogs containing modification at C-2 and at terminal olefinic positions)

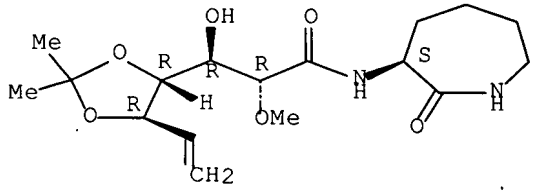
RN 870093-45-1 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-3-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-4,5-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



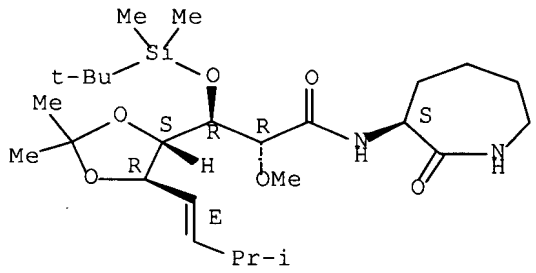
RN 870093-46-2 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-4,5-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 870093-48-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-3-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

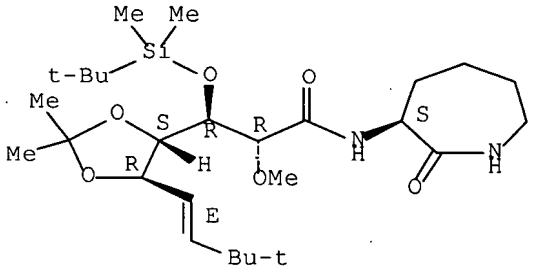
Absolute stereochemistry.
Double bond geometry as shown.



RN 870093-49-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-3-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-4,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

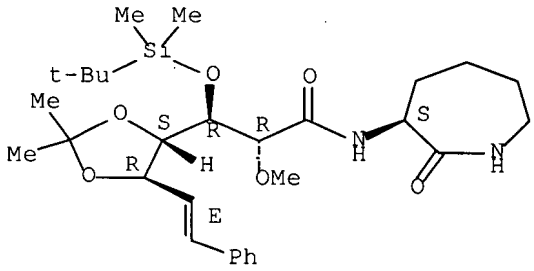
Absolute stereochemistry.

Double bond geometry as shown.



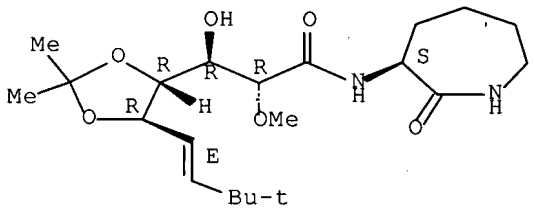
RN 870093-50-8 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-3-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-4,5-O-(1-methylethylidene)-7-phenyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 870093-67-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-4,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

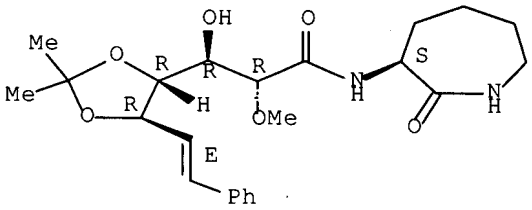
Absolute stereochemistry.
Double bond geometry as shown.



RN 870093-68-8 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-4,5-O-(1-methylethylidene)-7-phenyl-, (6E)- (9CI) (CA

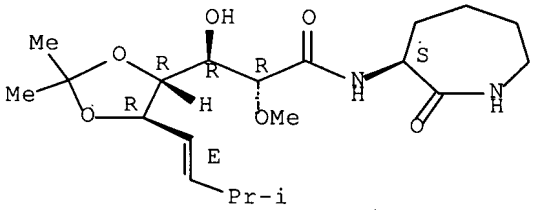
INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



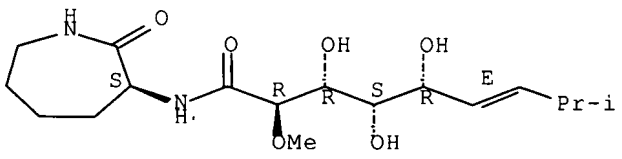
RN 870093-69-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



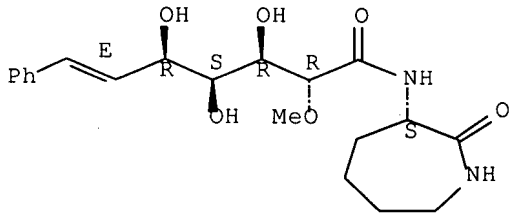
IT 118477-03-5P 844693-74-9P 870093-47-3P
870093-51-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of bengamide E and its analogs containing modification at C-2 and at terminal olefinic positions)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



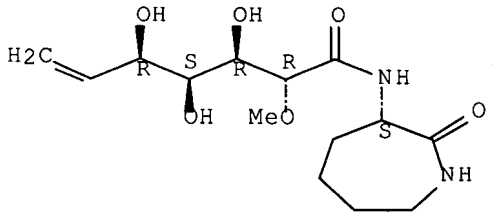
RN 844693-74-9 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-7-phenyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



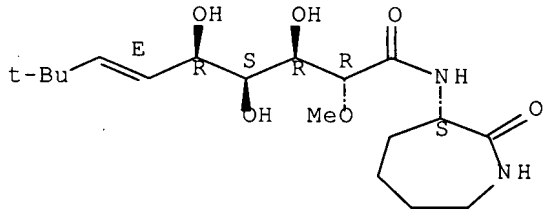
RN 870093-47-3 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 870093-51-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RE.CNT 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:429402 CAPLUS Full-text
DN 142:462366
TI Production of novel bengamides for cancer by fermentation with Myxococcus virescens ST200611
IN Hoffmann, Holger; Haag-Richter, Sabine; Kurz, Michael; Tietgen, Heiko
PA Aventis Pharma Deutschland G.m.b.H., Germany
SO PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005044803	A1	20050519	WO 2004-EP11244	20041008
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10349669	B3	20050525	DE 2003-10349669	20031024
	AU 2004287561	A1	20050519	AU 2004-287561	20041008
	CA 2543003	A1	20050519	CA 2004-2543003	20041008
	EP 1680405	A1	20060719	EP 2004-765884	20041008
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	CN 1871217	A	20061129	CN 2004-80030646	20041008
	BR 2004015529	A	20061226	BR 2004-15529	20041008
	JP 2007509084	T	20070412	JP 2006-535987	20041008
	US 2005171089	A1	20050804	US 2004-971228	20041022
	US 7153846	B2	20061226		
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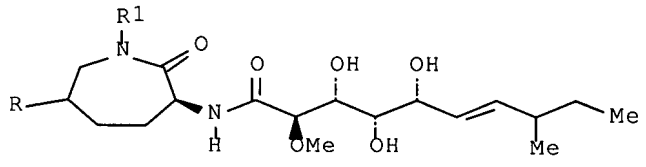
GI



I R=R1=H
II R=H, R1=Me
III R=OH, R1=H

AB The invention relates to bengamide derivs. which are formed by the microorganism Myxococcus virescens ST200611 (DSM 15898), during fermentation for use in the treatment of cancer, to medicaments containing bengamide

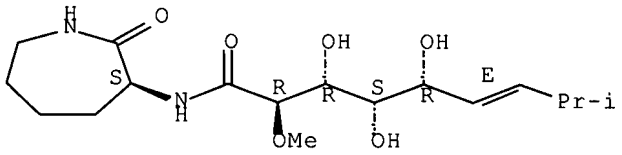
derivs., to a method for the production of bengamides (I, II, III) and their derivs., in addition to the microorganism Myxococcus virescens ST200611 (DSM 15898).

IT 118477-03-5P, Bengamide E 118477-04-6P, Bengamide F 851794-49-5DP, and physiol. salts of 851794-52-0DP, and physiol. salts of 851794-54-2DP, and physiol. salts of
RL: BMF (Bioindustrial manufacture); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(production of novel bengamides for cancer by fermentation with Myxococcus virescens ST200611)

RN 118477-03-5 CAPLUS

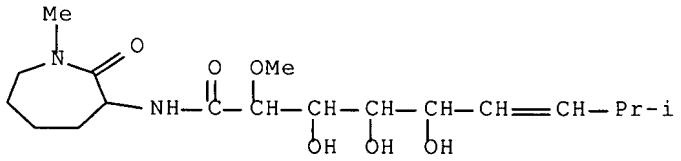
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 118477-04-6 CAPLUS

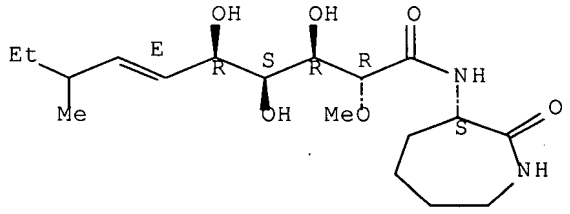
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



RN 851794-49-5 CAPLUS

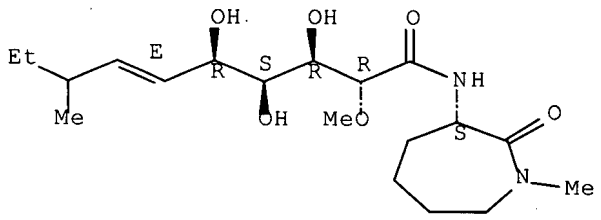
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



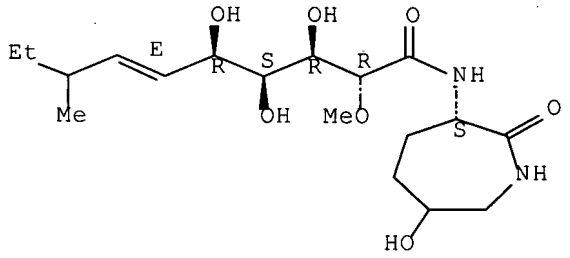
RN 851794-52-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



RN 851794-54-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-[(3S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E,8ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

Appl's

L10 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:141052 CAPLUS Full-text
DN 142:240712
TI Preparation and use of substituted lactams as anticancer agents
IN Bair, Kenneth Walter; Kinder, Frederick Ray, Jr.; Versace, Richard William
PA Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SO PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005014574	A1	20050217	WO 2004-EP8284	20040723
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004263287	A1	20050217	AU 2004-263287	20040723
	CA 2533335	A1	20050217	CA 2004-2533335	20040723
	EP 1651633	A1	20060503	EP 2004-763455	20040723
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	BR 2004012843	A	20060926	BR 2004-12843	20040723
	CN 1856486	A	20061101	CN 2004-80027798	20040723
	JP 2006528611	T	20061221	JP 2006-520809	20040723
	US 2006281731	A1	20061214	US 2006-565700	20060728
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	WO 2004-EP8284	W	20040723		

OS CASREACT 142:240712; MARPAT 142:240712
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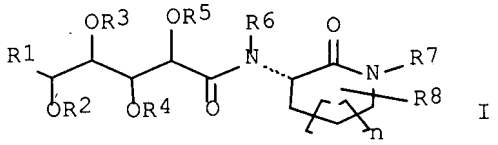

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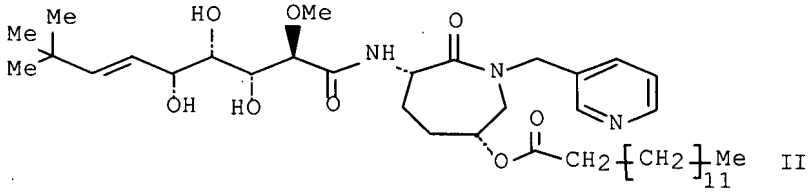

II

AB Substituted lactams, particularly caprolactam compds., such as I [n = 0-2, R1 = H, X-alkyl, X-alkylcarbonyl, X-alkenylene, X-alkynylene, X-cycloalkyl, X-cycloalkene, X-aryl; X = alkyl, cycloalkyl, ORa, SRa, NO2, halo, alkylamino; Ra = alkyl, aryl, OH, O-alkyl, halo; R2, R3, R4, R5 = H, alkyl; R5 = Ph, alkylphenyl; R2R4, R3R5 = acetal; R6 = H, alkyl; R7 = alkyl, Ph, pyridyl, cycloalkyl, N3, amino, etc.; R8 = H, halo, N3, alkyl, cycloalkyl, heterocyclyl, etc.], or a pharmaceutically acceptable salt thereof, were prepared as anticancer agents. Thus, caprolactam derivative II was prepared via a multistep synthetic sequence starting from α-D-glucoheptonic γ-lactone,

1,1-diiodo-2,2-dimethylpropane, (5R)-5-hydroxy-L-lysine, 3-chloromethylpyridine hydrochloride, and tetradecanoic acid. The prepared caprolactam derivs. showed an IC50 value in the range of 0.001 μM to 100 μM in the anchorage dependent growth monolayer assay (ADGMA) with MDA-MB-435 breast carcinoma line.

IT 661482-39-9P 844693-40-9P 844693-41-0P
844693-42-1P 844693-43-2P 844693-44-3P
844693-45-4P 844693-46-5P 844693-47-6P
844693-48-7P 844693-49-8P 844693-50-1P
844693-51-2P 844693-52-3P 844693-53-4P
844693-54-5P 844693-55-6P 844693-56-7P
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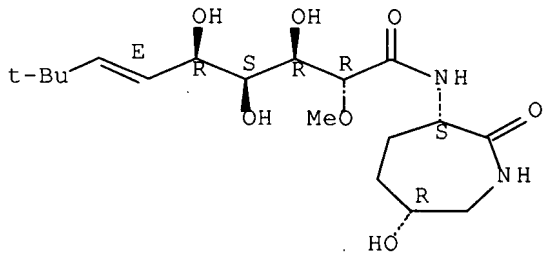
844693-90-9P 844693-91-0P 844693-92-1P
844693-94-3P 844693-95-4P 844693-97-6P
844693-98-7P 844693-99-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)(preparation and use of substituted caprolactams as anticancer agents)

RN 661482-39-9 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-, (6E)- (9CI) (CA INDEX NAME)

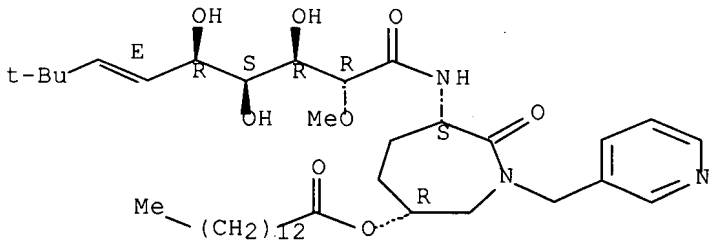
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-40-9 CAPLUS

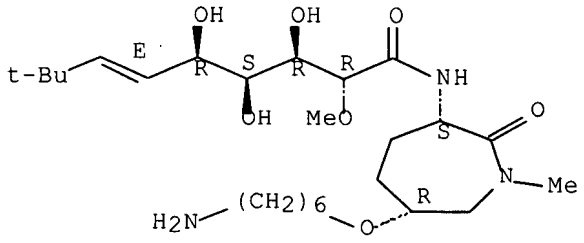
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1-(3-pyridinylmethyl)-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



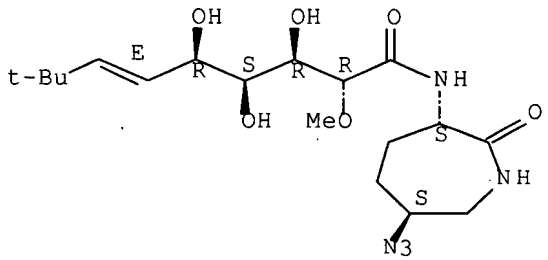
RN 844693-41-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(6-aminohexyl)oxy]hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-42-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-6-azidohexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

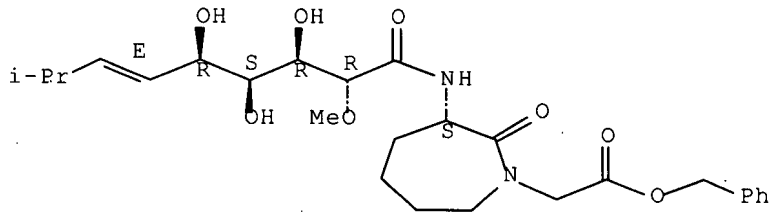
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-43-2 CAPLUS
CN 1H-Azepine-1-acetic acid, hexahydro-2-oxo-3-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

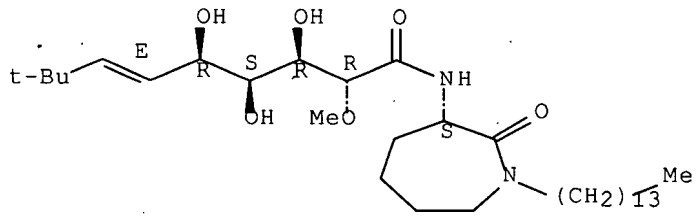
Absolute stereochemistry.

Double bond geometry as shown.



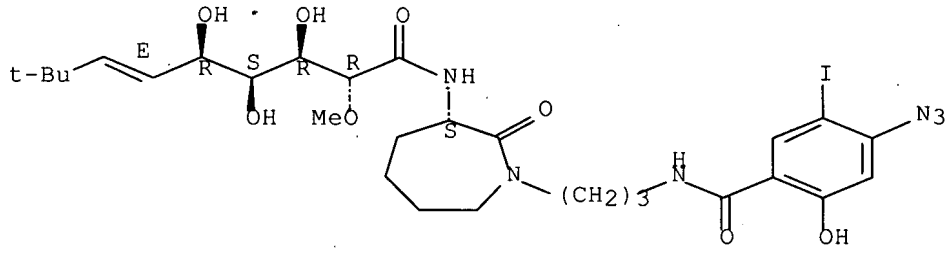
RN 844693-44-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1-tetradecyl-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-45-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-[3-[(4-azido-2-hydroxy-5-iodobenzoyl)amino]propyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

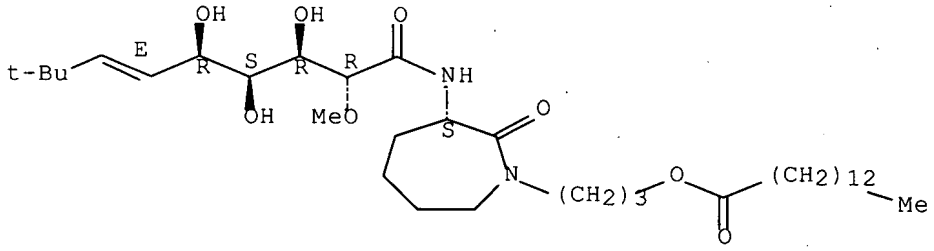
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-46-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-hexahydro-2-oxo-1-[3-[(1-oxotetradecyl)oxy]propyl]-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

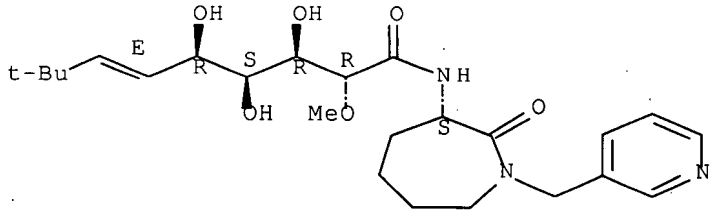
Absolute stereochemistry.

Double bond geometry as shown.



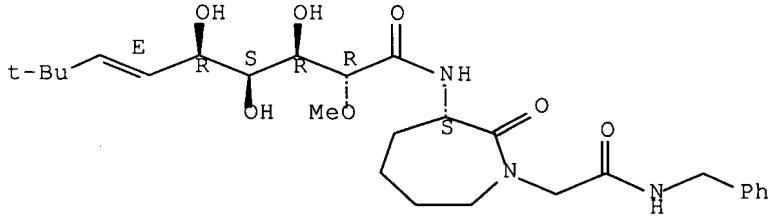
RN 844693-47-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1-(3-pyridinylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-48-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1-[2-oxo-2-[(phenylmethyl)amino]ethyl]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

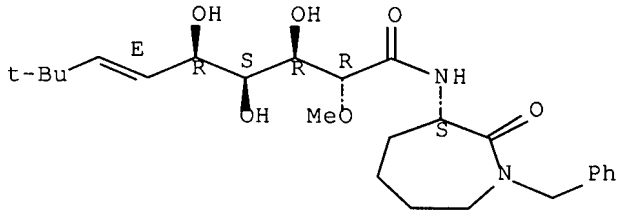
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-49-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1-(phenylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

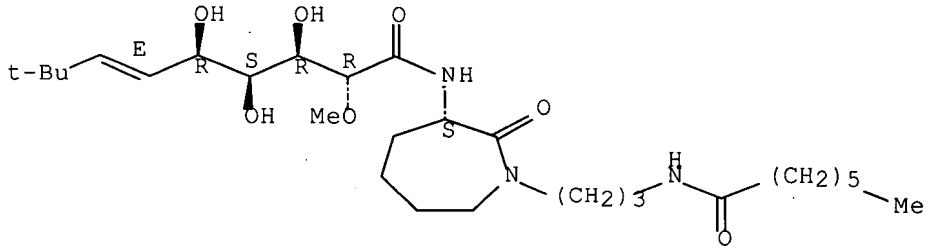
Absolute stereochemistry.

Double bond geometry as shown.



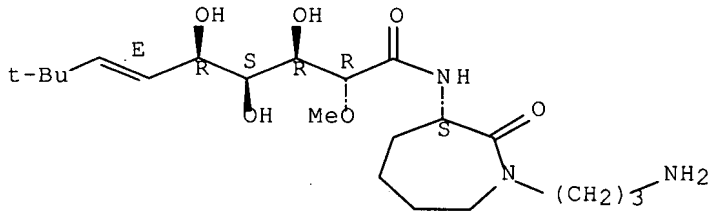
RN 844693-50-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1-[3-[(1-oxoheptyl)amino]propyl]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-51-2 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-(3-aminopropyl)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

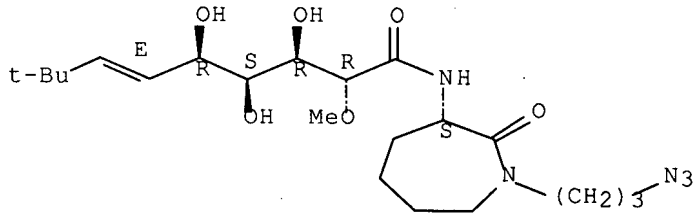
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-52-3 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-(3-azidopropyl)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

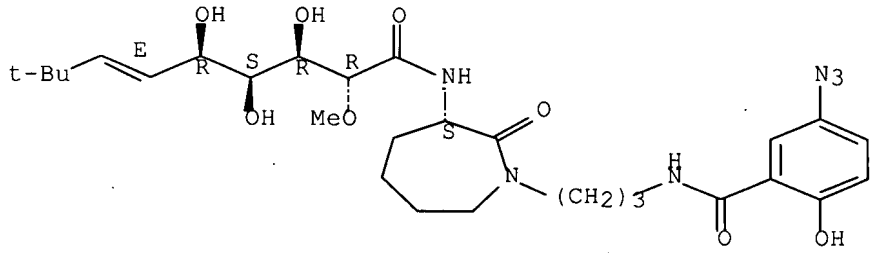
Absolute stereochemistry.

Double bond geometry as shown.



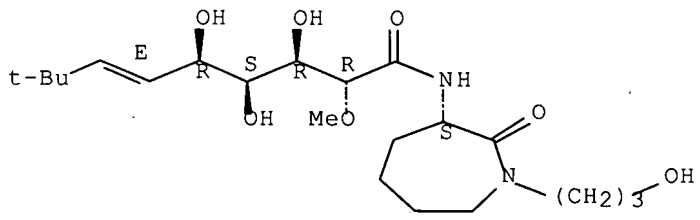
RN 844693-53-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S)-1-[3-[(5-azido-2-hydroxybenzoyl)amino]propyl]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-54-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-(3-hydroxypropyl)-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

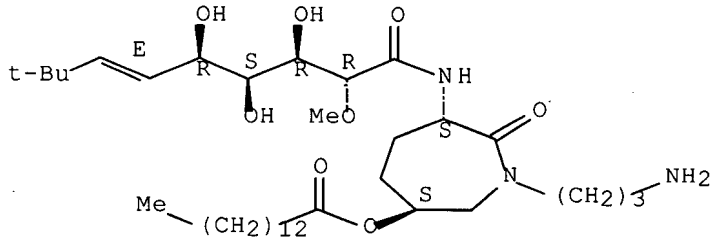
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-55-6 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-1-(3-aminopropyl)hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

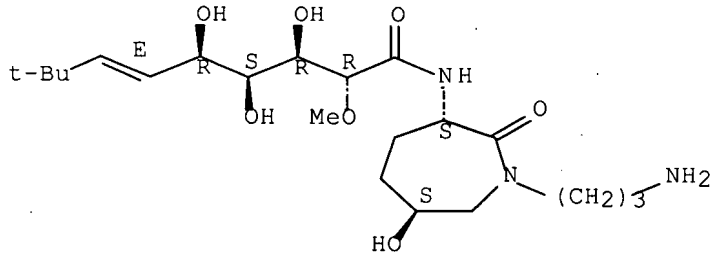
Absolute stereochemistry.

Double bond geometry as shown.



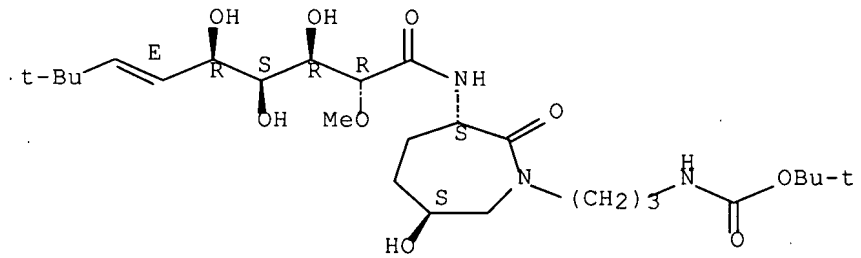
RN 844693-56-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-1-(3-aminopropyl)hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



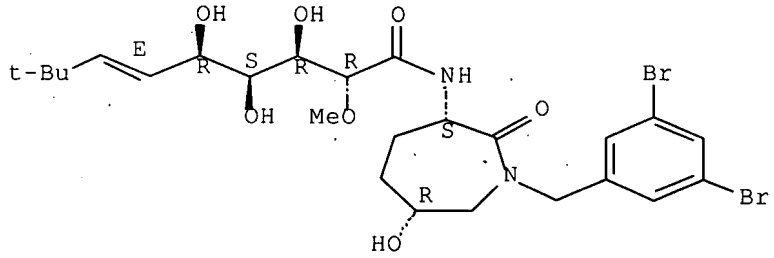
RN 844693-57-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-1-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



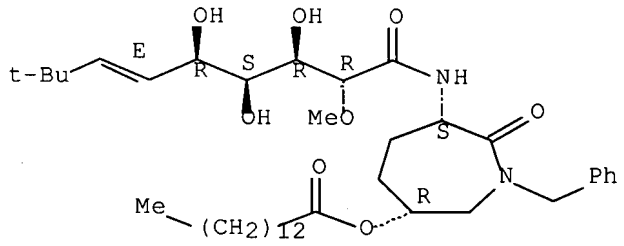
RN 844693-58-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-1-[(3,5-dibromophenyl)methyl]hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



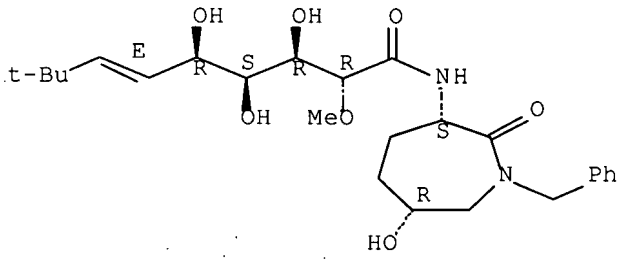
RN 844693-59-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1-(phenylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-60-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1-(phenylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

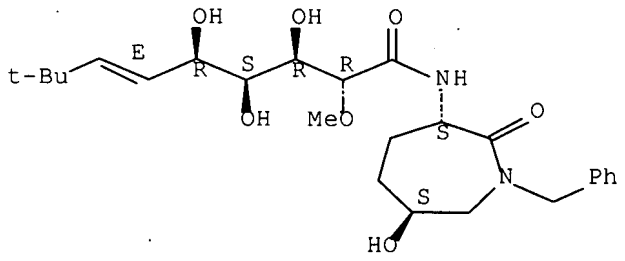
Absolute stereochemistry.
Double bond geometry as shown.



RN 844693-61-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-

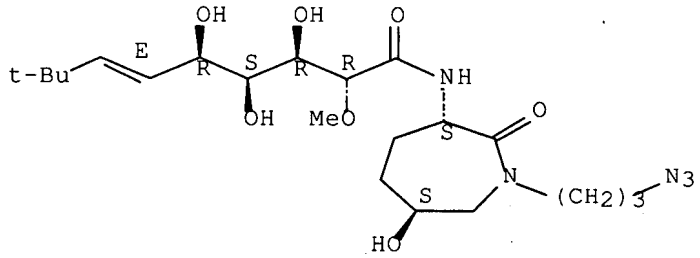
2-oxo-1-(phenylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



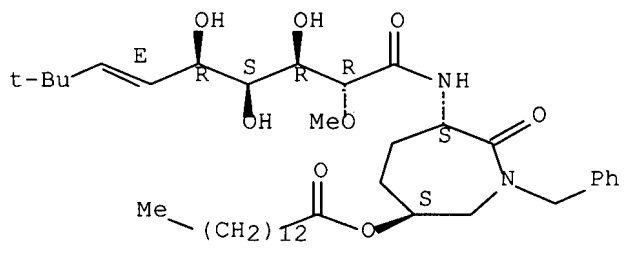
RN 844693-62-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-1-(3-azidopropyl)hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



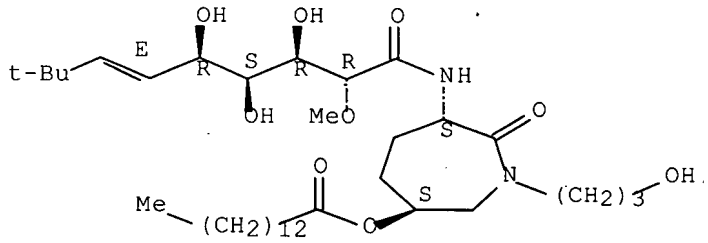
RN 844693-63-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1-(phenylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



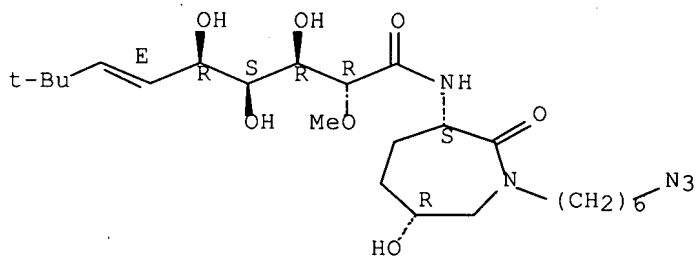
RN 844693-64-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-(3-hydroxypropyl)-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



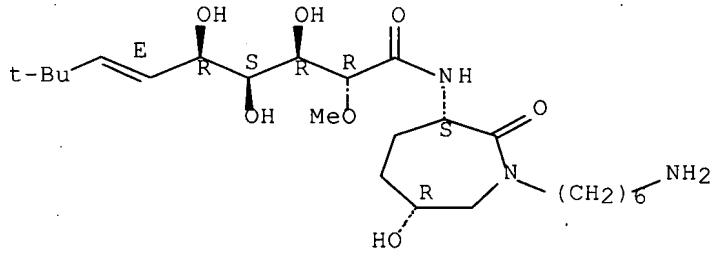
RN 844693-65-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-1-(6-azidohexyl)hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



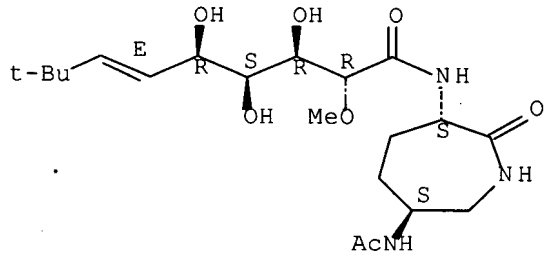
RN 844693-66-9 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-1-(6-aminohexyl)hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



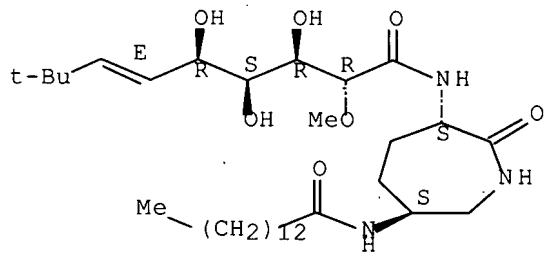
RN 844693-67-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-6-(acetylamino)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



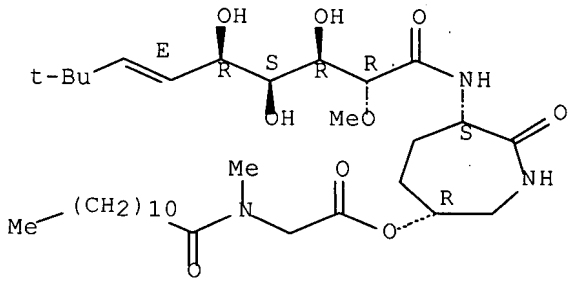
RN 844693-68-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)amino]-1H-azepin-3-yl]-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



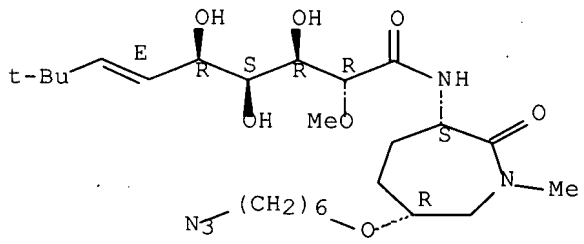
RN 844693-69-2 CAPLUS
CN Glycine, N-methyl-N-(1-oxododecyl)-, (3R,6S)-hexahydro-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



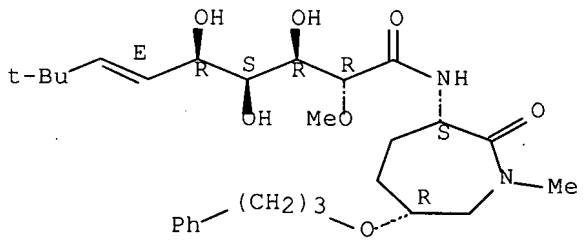
RN 844693-70-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(6-azidohexyl)oxy]hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



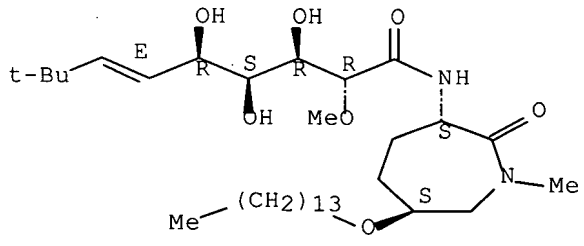
RN 844693-71-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-1-methyl-2-oxo-6-(3-phenylpropoxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



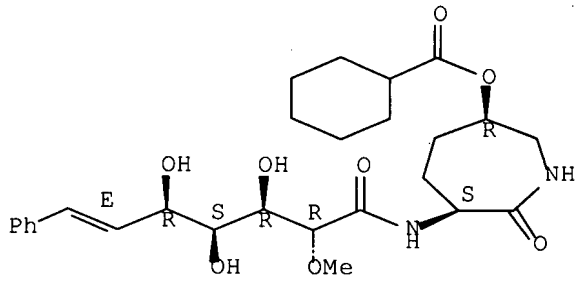
RN 844693-72-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-(tetradecyloxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



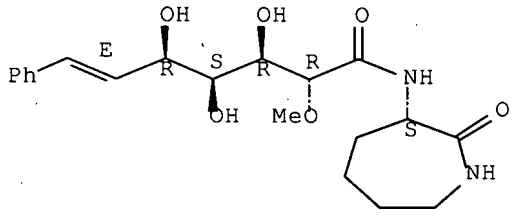
RN 844693-73-8 CAPLUS
CN D-gulo-Hept-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7-dideoxy-2-O-methyl-7-phenyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



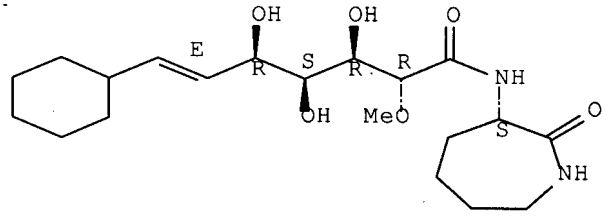
RN 844693-74-9 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-7-phenyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



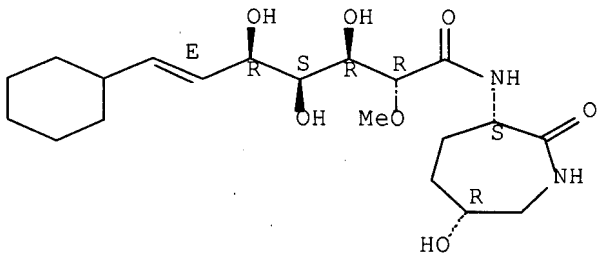
RN 844693-75-0 CAPLUS
CN D-gulo-Hept-6-enonamide, 7-cyclohexyl-6,7-dideoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



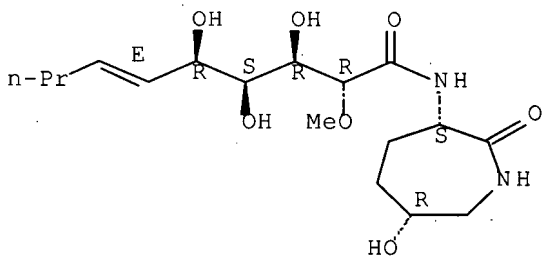
RN 844693-76-1 CAPLUS
CN D-gulo-Hept-6-enonamide, 7-cyclohexyl-6,7-dideoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



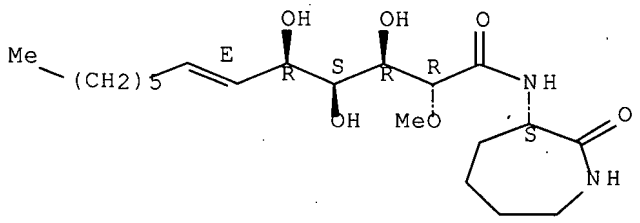
RN 844693-77-2 CAPLUS
CN 6-Decenamide, N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-3,4,5-trihydroxy-2-methoxy-, (2R,3R,4S,5R,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



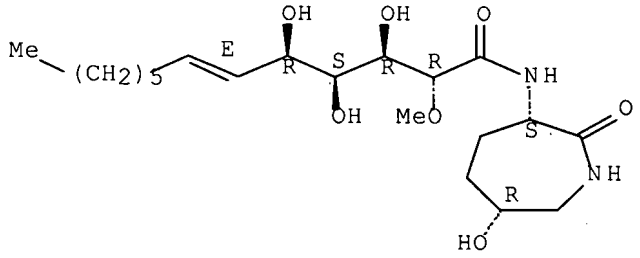
RN 844693-78-3 CAPLUS
CN 6-Tridecenamide, N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-3,4,5-trihydroxy-2-methoxy-, (2R,3R,4S,5R,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



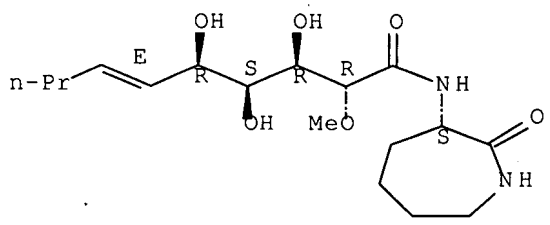
RN 844693-79-4 CAPLUS
CN 6-Tridecenamide, N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-3,4,5-trihydroxy-2-methoxy-, (2R,3R,4S,5R,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



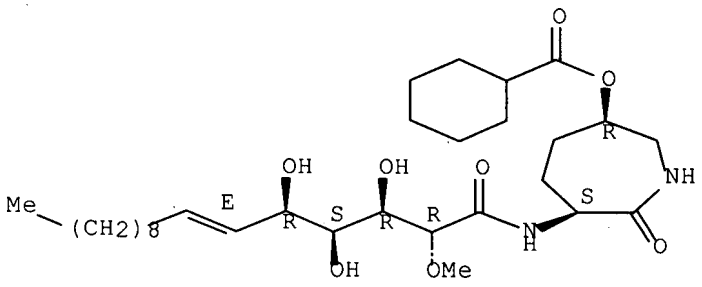
RN 844693-80-7 CAPLUS
CN 6-Decenamide, N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-3,4,5-trihydroxy-2-methoxy-, (2R,3R,4S,5R,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



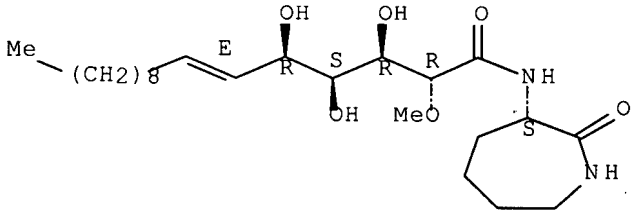
RN 844693-81-8 CAPLUS
CN Cyclohexanecarboxylic acid, (3R,6S)-hexahydro-7-oxo-6-[[(2R,3R,4S,5R,6E)-3,4,5-trihydroxy-2-methoxy-1-oxo-6-hexadecenyl]amino]-1H-azepin-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



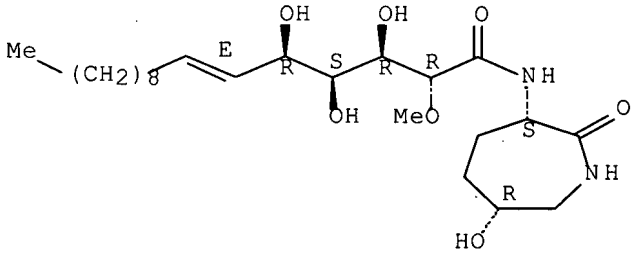
RN 844693-82-9 CAPLUS
CN 6-Hexadecenamide, N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-3,4,5-trihydroxy-2-methoxy-, (2R,3R,4S,5R,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



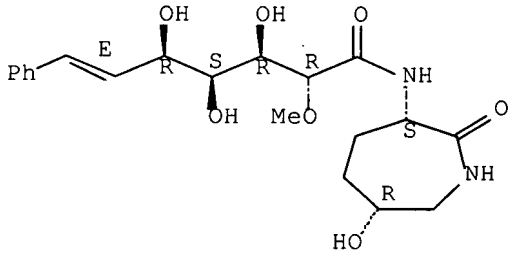
RN 844693-83-0 CAPLUS
CN 6-Hexadecenamide, N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-3,4,5-trihydroxy-2-methoxy-, (2R,3R,4S,5R,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



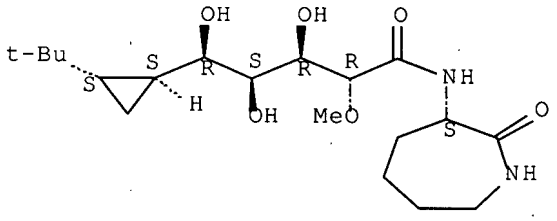
RN 844693-84-1 CAPLUS
CN D-gulo-Hept-6-enonamide, 6,7-dideoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-2-O-methyl-7-phenyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



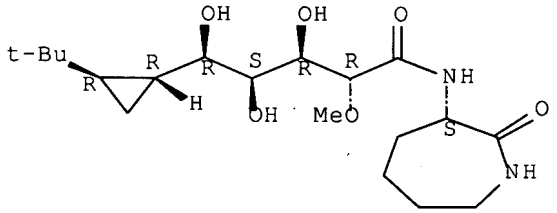
RN 844693-85-2 CAPLUS
CN L-Lyxonamide, 5-C-[(1S,2S)-2-(1,1-dimethylethyl)cyclopropyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



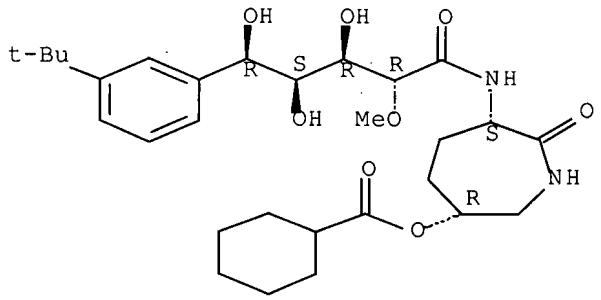
RN 844693-86-3 CAPLUS
CN L-Lyxonamide, 5-C-[(1R,2R)-2-(1,1-dimethylethyl)cyclopropyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



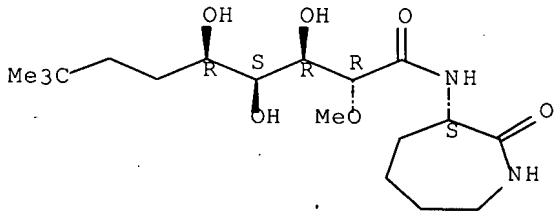
RN 844693-87-4 CAPLUS
CN L-Lyxonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-5-C-[3-(1,1-dimethylethyl)phenyl]-2-O-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



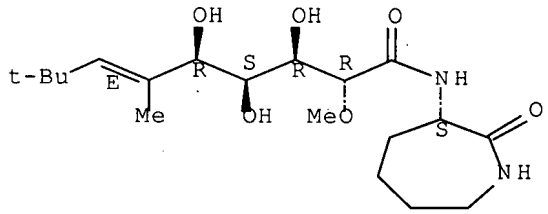
RN 844693-88-5 CAPLUS
CN D-gulo-Nononamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



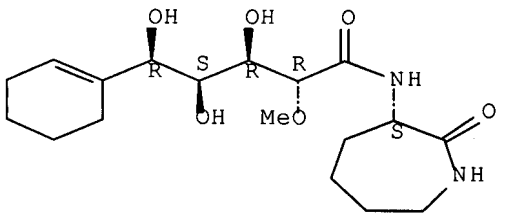
RN 844693-89-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-6,8,8-trimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



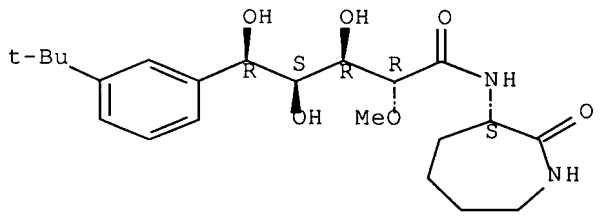
RN 844693-90-9 CAPLUS
CN L-Lyxonamide, 5-C-1-cyclohexen-1-yl-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



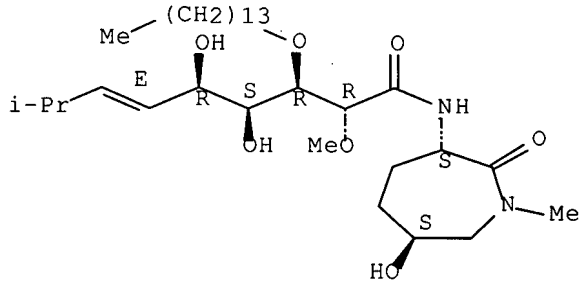
RN 844693-91-0 CAPLUS
CN L-Lyxonamide, 5-C-[3-(1,1-dimethylethyl)phenyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-2-O-methyl-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



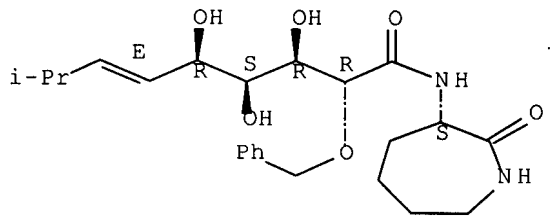
RN 844693-92-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-3-O-tetradecyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



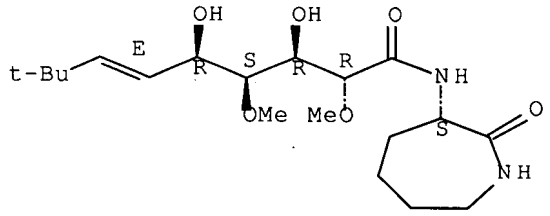
RN 844693-94-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



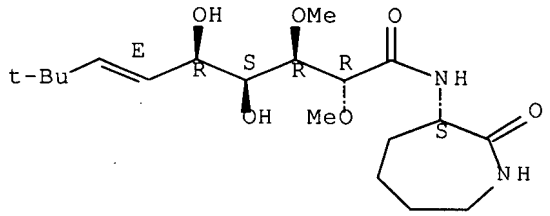
RN 844693-95-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2,4-di-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



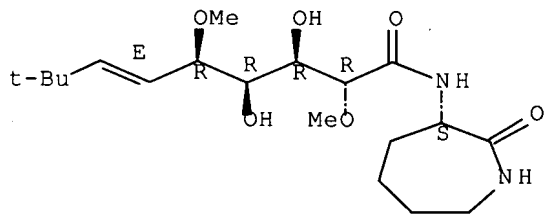
RN 844693-97-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2,3-di-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



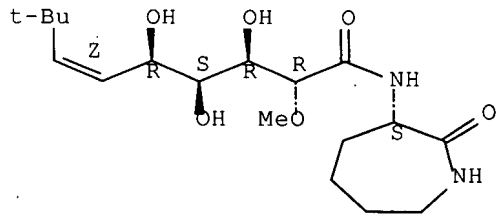
RN 844693-98-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2,5-di-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



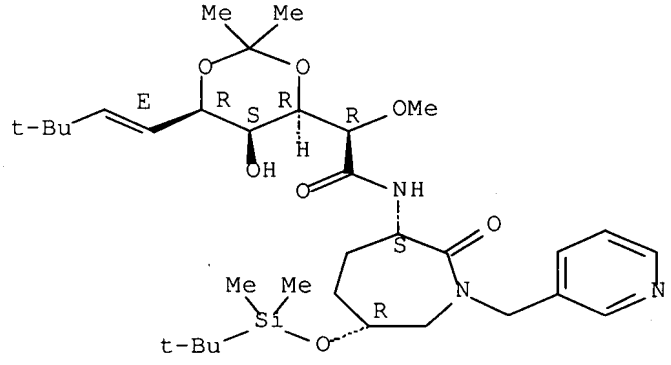
RN 844693-99-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



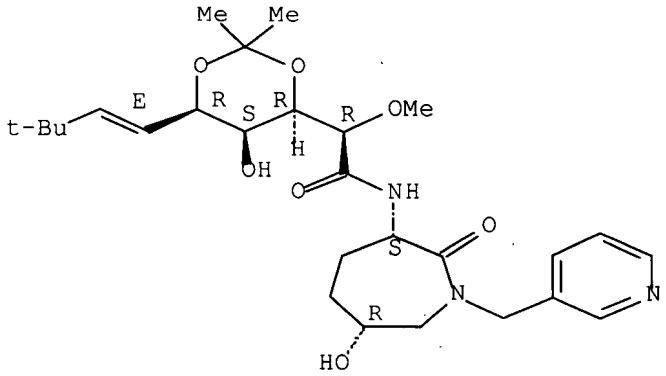
IT 844694-06-0P 844694-07-1P 844694-09-3P
844694-15-1P 844694-18-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and use of substituted caprolactams as anticancer agents)
RN 844694-06-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-oxo-1-(3-pyridinylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



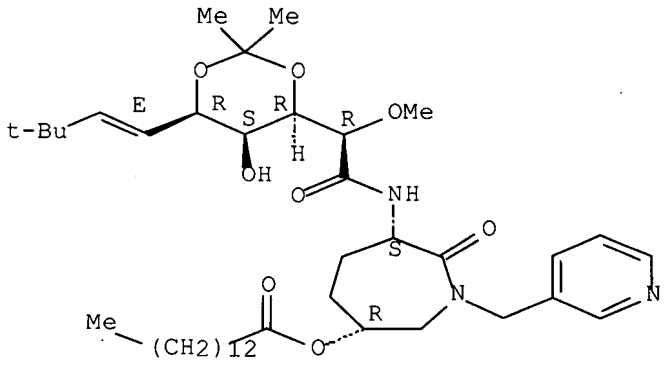
RN 844694-07-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1-(3-pyridinylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



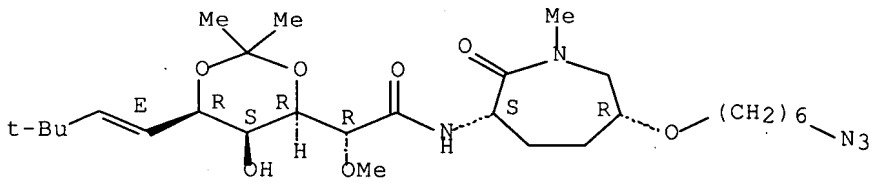
RN 844694-09-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1-(3-pyridinylmethyl)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 844694-15-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(6-azidohexyl)oxy]hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

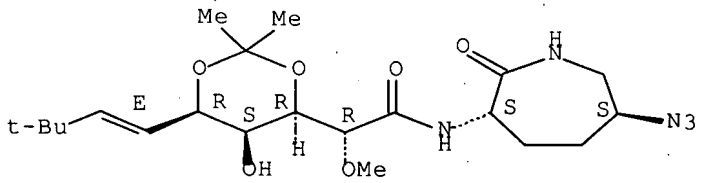
Absolute stereochemistry.
Double bond geometry as shown.



RN 844694-18-4 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6S)-6-azidohexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

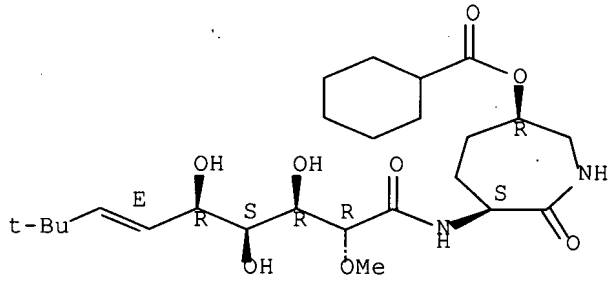
Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

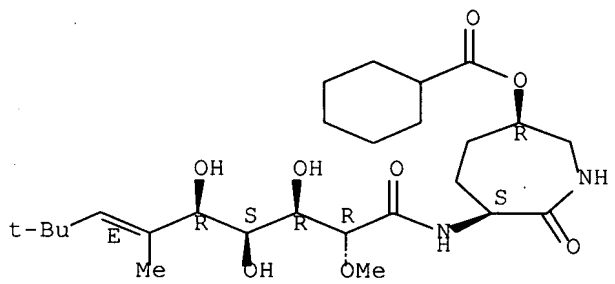
L10 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1130504 CAPLUS Full-text
DN 143:318447
TI Depletion of methionine aminopeptidase 2 does not alter cell response to fumagillin or bengamides. [Erratum to document cited in CA141:046873]
AU Kim, Sunkyu; LaMontagne, Kenneth; Sabio, Michael; Sharma, Sushil; Versace, Richard W.; Yusuff, Naeem; Phillips, Penny E.
CS Novartis Pharmaceuticals, East Hanover, NJ, 07936, USA
SO Cancer Research (2004), 64(24), 9230
CODEN: CNREA8; ISSN: 0008-5472
PB American Association for Cancer Research
DT Journal
LA English
AB On page 2984, "Cell and Enzyme Assays" section, the text near the end of the section should read: "The targeting sequence was AAUGCCGGUGACACAACAGUA (Dharmacon Research). The control mismatch sequence was AAUGCCGGCGCUACAACAGUA.".
IT 270902-51-7, LAF 389 708277-86-5, LBM 648
RL: PAC (Pharmacological activity); BIOL (Biological study)
(depletion of methionine aminopeptidase 2 does not alter cell response to fumagillin or bengamides (Erratum))
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

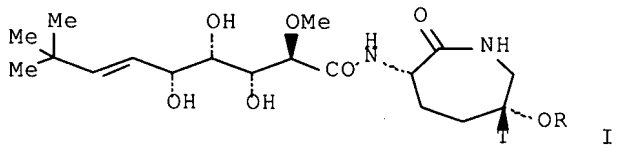


RN 708277-86-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-6,8,8-trimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



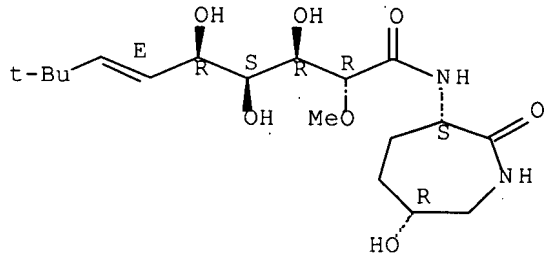
L10 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:859470 CAPLUS Full-text
DN 142:355446
TI Enzymatic hydrolysis of LAF 389
AU Bordeaux, Kirk; Ray, Tapan
CS Isotope Laboratory Dept. of Preclinical Safety, Novartis Pharmaceuticals Corporation, East Hanover, NJ, 07936, USA
SO Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 8th, Boston, MA, United States, June 1-5, 2003 (2004), Meeting Date 2003, 409-412. Editor(s): Dean, Dennis C.; Filer, Crist N.; McCarthy, Keith E. Publisher: John Wiley & Sons Ltd., Chichester, UK.
CODEN: 69FZAZ; ISBN: 0-470-86365-X
DT Conference
LA English
OS CASREACT 142:355446
GI



I

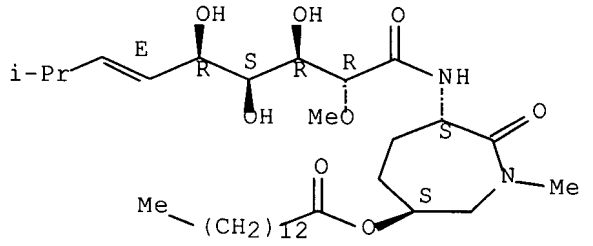
AB Bengamide B is a novel marine natural product with impressive in vitro and in vivo antitumor activity. SAR studies have shown that the in vitro potency of the bengamide B series is dependent on the presence of the metabolically labile ester moiety. These data suggest that the ester moiety may serve to facilitate cellular penetration. After the evaluation of a large number of analogs, LAF 389 was chosen as the drug candidate for further evaluation. Both [3H]-LAF 389 I (R = cyclohexylcarbonyl) and [3H]-LAF 153 I (R = H) were required to support further biol. profiling and development of LAF389. The chemical hydrolysis of radiolabeled LAF 389 gave many byproducts that could not be easily purified. The use of ThermoCat QuickScreen Ester Hydrolysis Kit made it possible to identify an esterase that was capable of hydrolyzing LAF 389 cleanly to LAF 153.
IT 661482-39-9P, LAF 153
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzymic hydrolysis of [3H]-LAF 389)
RN 661482-39-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



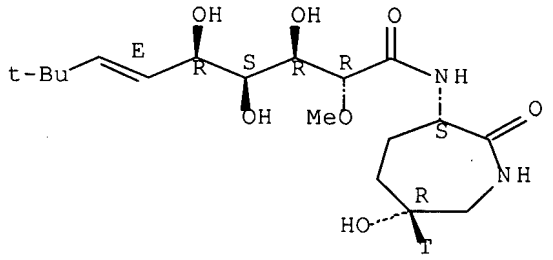
IT 104947-69-5DP, Bengamide B, analogs 848844-09-7P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(enzymic hydrolysis of [3H]-LAF 389)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 848844-09-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl-6-t]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



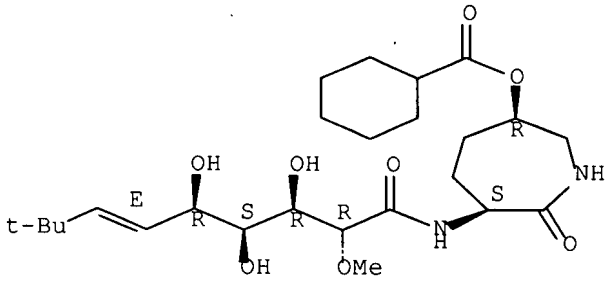
IT 270902-51-7, LAF 389 848844-06-4
RL: RCT (Reactant); RACT (Reactant or reagent)

(enzymic hydrolysis of [3H]-LAF 389)

RN 270902-51-7 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

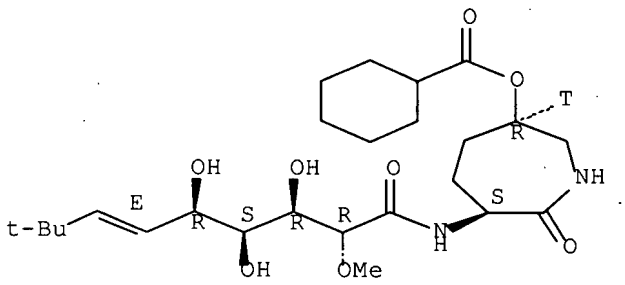
Absolute stereochemistry.
Double bond geometry as shown.



RN 848844-06-4 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl-6-t]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

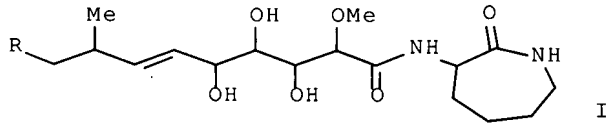
Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:778856 CAPLUS Full-text
DN 141:273024
TI Compound N-9011A, its microbial manufacture, and agrochemical pesticides containing it or its analog
IN Tomie, Tetsuya; Aikawa, Junko; Takii, Shinji; Seki, Tatsuya
PA Noyaku Bio Technology Kaihatsu Gijutsu Kenkyu Kumiai, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2004262793	A	20040924	JP 2003-52944	20030228
PRAI	JP 2003-52944		20030228		

GI



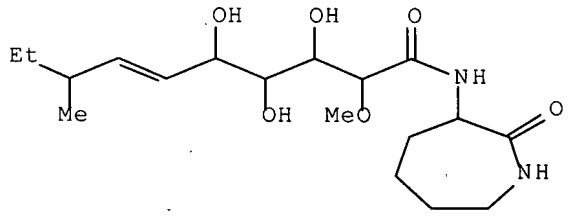
I

AB Agrochems., useful as insecticides, herbicides, and microbicides, contain N-9011A (I; R = Me) or N-9011B (I; R = H). Myxococcus sp. Number 0187 was cultured to produce N-9011A and B, which showed ≥60% control of Plutella xylostella at 25 ppm.

IT 757222-35-8P, N 9011A 757222-39-2P, N 9011B
RL: AGR (Agricultural use); BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation); USES (Uses)
(agrochem. pesticides containing N-9011A or B manufactured with Myxococcus sp.)

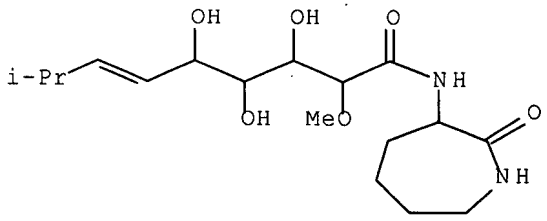
RN 757222-35-8 CAPLUS
CN Non-6-enonamide, 6,7,8,9-tetradeoxy-8-ethyl-N-(hexahydro-2-oxo-1H-azepin-3-yl)-2-O-methyl- (9CI) (CA INDEX NAME)

Double bond geometry unknown.
Currently available stereo shown.



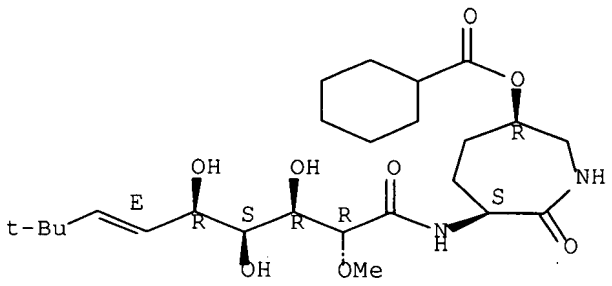
RN 757222-39-2 CAPLUS
CN Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl- (9CI) (CA INDEX NAME)

Double bond geometry unknown.
Currently available stereo shown.


OH
OH
O
i-Pr
NH
OH
MeO
O
NH

L10 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:695101 CAPLUS Full-text
DN 142:106282
TI Molecular Approaches to Discover Marine Natural Product Anticancer Leads - An Update from a Drug Discovery Group Collaboration
AU Crews, Phillip; Gerwick, William; Schmitz, Francis; France, Dennis; Bair, Kenneth; Wright, Amy; Hallock, Yali
CS Department of Chemistry and Biochemistry & Institute of Marine Sciences, Univ. California, Santa Cruz, CA, 95064, USA
SO Pharmaceutical Biology (Lisse, Netherlands) (2003), 41(Suppl. 1), 39-52
CODEN: PHBIFC; ISSN: 1388-0209
PB Taylor & Francis The Netherlands
DT Journal; General Review
LA English
AB A review. This paper outlines the results of a collaborative program begun in 1990 under the NIH National Cooperative Drug Discovery Group (NCDDG) program. It involves the unified research of a multi-institutional group from both academic and corporate labs. Our working hypothesis is that targets identified through basic mol. and cell biol. studies are relevant for the treatment of human cancers. Thus, a broad range of primary biochem. assays have guided the examination of exts. obtained from marine organisms (both collected and cultured) and purified marine natural products. The goal is to discover small mols. effective against these biol. targets. An ever-changing panel of assays focus on a number of cancer relevant targets associated with the cell cycle, signal transduction, angiogenesis or apoptosis. A massive library of materials has been assembled for evaluation of the screens and it consists of more than 900 compds. and 16,000 exts. We believe that these samples have enormous potential for chemodiversity and progress to date supports this contention. The first part of the paper focuses on highlights from the period 1995-1999. The two most important developments were that the bengamide and the psammaplin families provided important insights leading to the development of two compds., LAF-389 and NVP-LAQ824. These were both advanced to Phase I anti-cancer clin. trials. A sampling of recent discoveries, including current leads in development is also discussed. Attention then turns to new technologies and strategies aimed at shortening the time interval from an initial lead candidate discovery to assessment of its future therapeutic potential.
IT 270902-51-7, LAF 389
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(LAF-389 developed from bengamide and psammaplin family is advanced to phase I clin. trial in treating cancer patient)
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

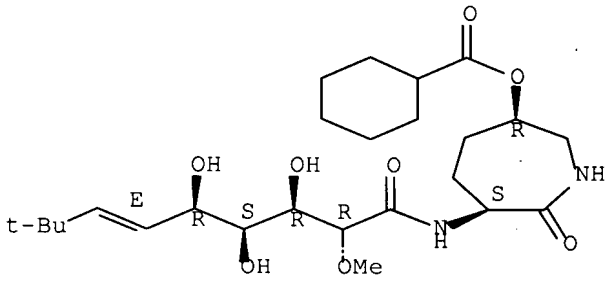
Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

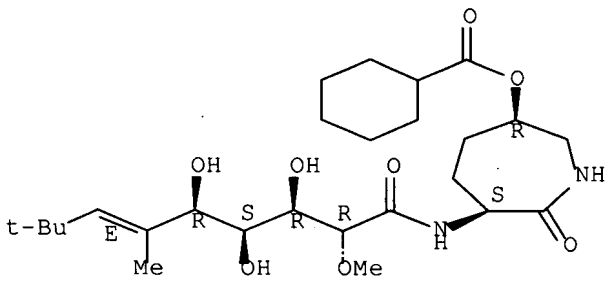
L10 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:363227 CAPLUS Full-text
DN 141:46873
TI Depletion of Methionine Aminopeptidase 2 Does Not Alter Cell Response to Fumagillin or Bengamides
AU Kim, Sunkyu; LaMontagne, Kenneth; Sabio, Michael; Sharma, Sushil; Versace, Richard W.; Yusuff, Naeem; Phillips, Penny E.
CS Novartis Pharmaceuticals, East Hanover, NJ, 07936, USA
SO Cancer Research (2004), 64(9), 2984-2987
CODEN: CNREA8; ISSN: 0008-5472
PB American Association for Cancer Research
DT Journal
LA English
AB Inhibition of endothelial cell growth by fumagillin has been assumed to be mediated by inhibition of the mol. target methionine aminopeptidase 2 (MetAp2). New data show that depletion of MetAp2 by siRNA does not inhibit endothelial cell growth. Moreover, MetAp2-depleted endothelial cells remain responsive to inhibition by either fumagillin or a newly identified MetAp2 enzyme inhibitor. These data suggest that MetAp2 function is not required for endothelial cell proliferation.
IT 270902-51-7, LAF 389 708277-86-5, LBM 648
RL: PAC (Pharmacological activity); BIOL (Biological study)
(depletion of methionine aminopeptidase 2 does not alter cell response to fumagillin or bengamides)
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



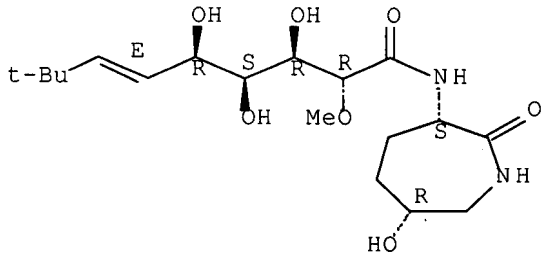
RN 708277-86-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-6,8,8-trimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:995068 CAPLUS Full-text
DN 140:192464
TI Proteomics-based Target Identification: Bengamides as a new class of methionine aminopeptidase inhibitors
AU Towbin, Harry; Bair, Kenneth W.; DeCaprio, James A.; Eck, Michael J.; Kim, Sunkyu; Kinder, Frederick R.; Morollo, Anthony; Mueller, Dieter R.; Schindler, Patrick; Song, Hyun Kyu; van Oostrum, Jan; Versace, Richard W.; Voshol, Hans; Wood, Jeanette; Zabludoff, Sonya; Phillips, Penny E.
CS Novartis Pharma AG, Basel, CH-4036, Switz.
SO Journal of Biological Chemistry (2003), 278(52), 52964-52971
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
AB LAF389 is a synthetic analog of bengamides, a class of marine natural products that produce inhibitory effects on tumor growth in vitro and in vivo. A proteomics-based approach has been used to identify signaling pathways affected by bengamides. LAF389 treatment of cells resulted in altered mobility of a subset of proteins on two-dimensional gel electrophoresis. Detailed anal. of one of the proteins, 14-3-3γ, showed that bengamide treatment resulted in retention of the amino-terminal methionine, suggesting that bengamides directly or indirectly inhibited methionine aminopeptidases (MetAps). Both known MetAps are inhibited by LAF389. Short interfering RNA suppression of MetAp2 also altered amino-terminal processing of 14-3-3γ. A high resolution structure of human MetAp2 co-crystallized with a bengamide shows that the compound binds in a manner that mimics peptide substrates. Addnl., the structure reveals that three key hydroxyl groups on the inhibitor coordinate the di-cobalt center in the enzyme active site.
IT 661482-39-9D, co-crystallized with MetAp2
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(proteomics-based target identification of bengamides as methionine aminopeptidase inhibitors)
RN 661482-39-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



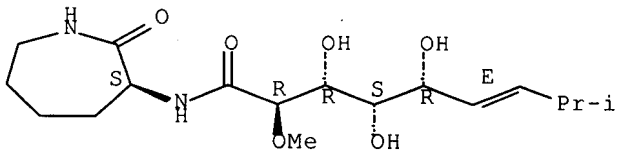
IT 118477-03-5P, Bengamide E
RL: DMA (Drug mechanism of action); NPO (Natural product occurrence); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(proteomics-based target identification of bengamides as methionine

aminopeptidase inhibitors)

RN 118477-03-5 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 270902-51-7P, LAF 389

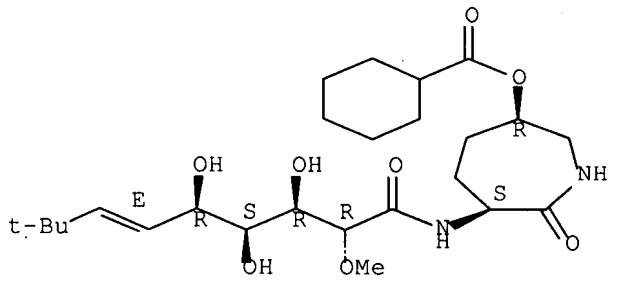
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(proteomics-based target identification of bengamides as methionine aminopeptidase inhibitors)

RN 270902-51-7 CAPLUS

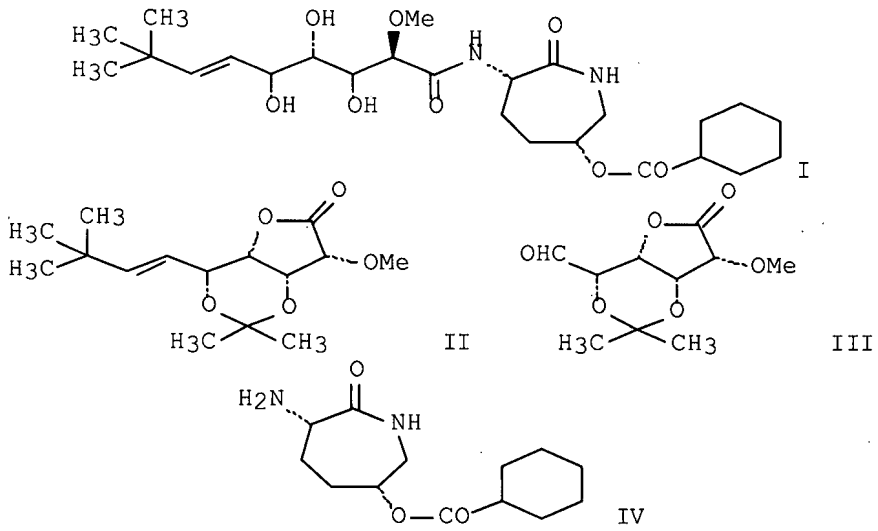
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



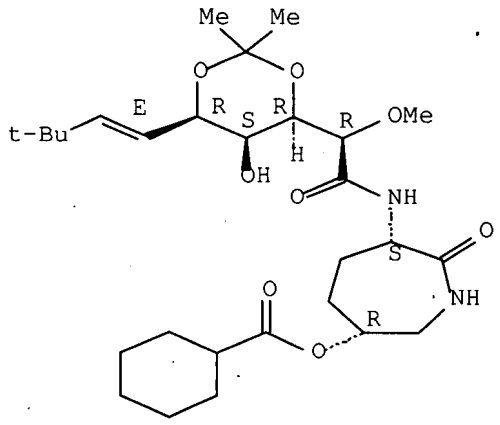
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:743312 CAPLUS Full-text
DN 139:350890
TI An Expedient Synthesis of LAF389, a Bengamide B Analogue
AU Xu, David D.; Waykole, Liladhar; Calienni, John V.; Ciszewski, Lech; Lee, George T.; Liu, Wenming; Szewczyk, Joanna; Vargas, Kevin; Prasad, Kapa; Repic, Oljan; Blacklock, Thomas J.
CS Process R & D, Chemical and Analytical Development, Novartis Institute for Biomedical Research, East Hanover, NJ, 07936, USA
SO Organic Process Research & Development (2003), 7(6), 856-865
CODEN: OPRDFK; ISSN: 1083-6160
PB American Chemical Society
DT Journal
LA English
OS CASREACT 139:350890
GI



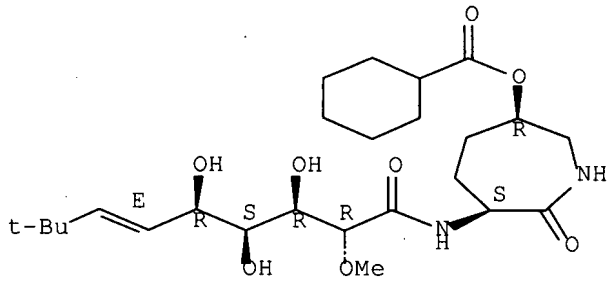
AB An optimized, convergent, safe synthesis of LAF389 (I), an anticancer agent analogous to bengamide B, is described. Starting from D-glycero-D-gulo-heptonic acid γ-lactone, lactone II was constructed in five steps. Major improvements were made in the preparation of the aldehyde precursor III and its subsequent olefination to give II via a modified Julia protocol. This olefination was significantly improved by using TMSCl as an additive. The second fragment, ε-caprolactam IV, was obtained in two one-pot operations from (5R)-5-hydroxy-L-lysine. Finally, ring opening of II with IV using sodium 2-Et hexanoate (Na-EH) gave I in a protected form, which was deprotected to give I.
IT 270902-71-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(expedient synthesis of LAF389, a bengamide B analog)
RN 270902-71-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 270902-51-7P, LAF 389
RL: SPN (Synthetic preparation); PREP (Preparation)
(expedient synthesis of LAF389, a bengamide B analog)
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

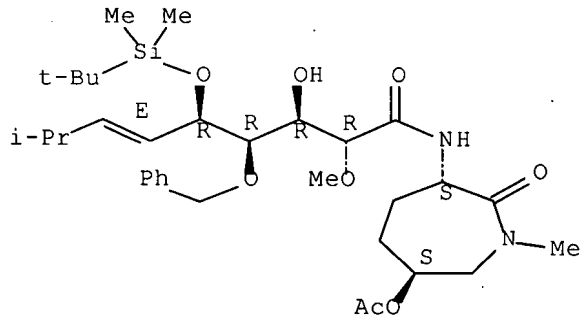
Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

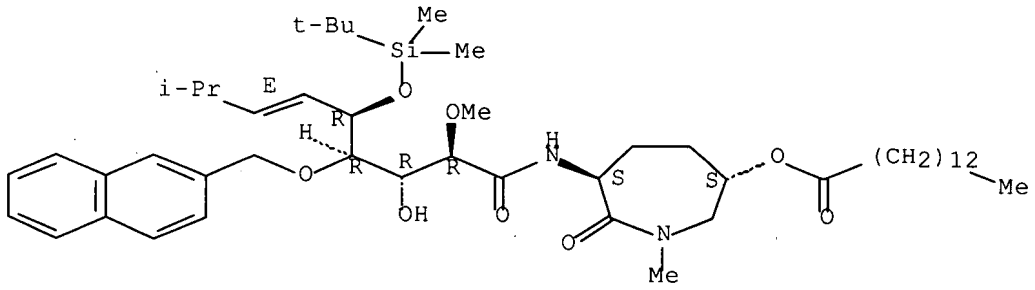
L10 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:69877 CAPLUS Full-text
DN 139:53277
TI The development of a convergent and efficient enantioselective synthesis of the bengamides via a common polyol intermediate
AU Boeckman, Robert K., Jr.; Clark, Tammy J.; Shook, Brian C.
CS Department of Chemistry, University of Rochester, Rochester, NY, 14627-0216, USA
SO Helvetica Chimica Acta (2002), 85(12), 4532-4560
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
OS CASREACT 139:53277
AB An efficient, general synthetic route to the bengamide family of antitumor agents from a common polyol thioester is described. Consecutive aldol condensations afford the protected polyol thioester side chain suitable for coupling to the bengamides. A novel chiral-phase-transfer-catalyzed enantioselective alkylation affords the properly functionalized caprolactams required for the synthesis of more complex members of the bengamide family. Use of the Me 2-naphthyl either protecting group, compatible with the boron Lewis acids required for enantioselective aldol condensation, allows direct access to all the bengamides.
IT 442913-34-0P 442913-40-8P 442913-43-1P
442913-44-2P 547742-45-0P 547742-46-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(convergent and efficient enantioselective synthesis of bengamides via polyol intermediate)
RN 442913-34-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-6-(acetyloxy)hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



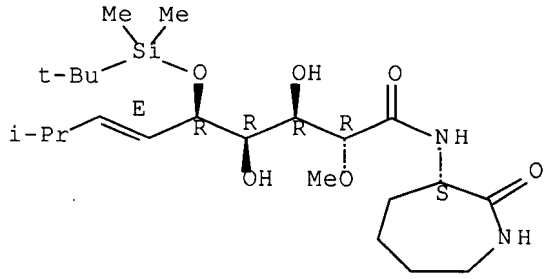
RN 442913-40-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(2-naphthalenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



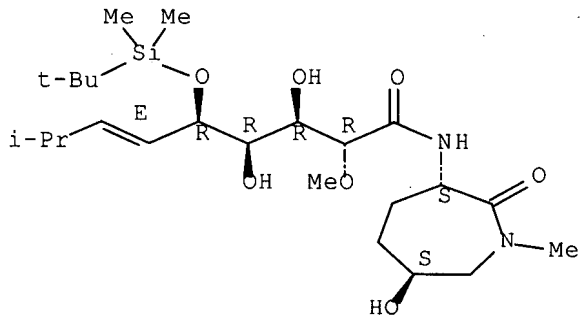
RN 442913-43-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 442913-44-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

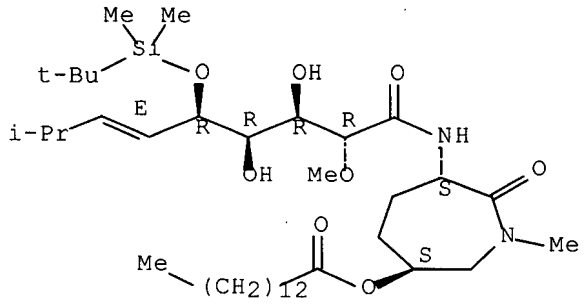
Absolute stereochemistry.
Double bond geometry as shown.



RN 547742-45-0 CAPLUS

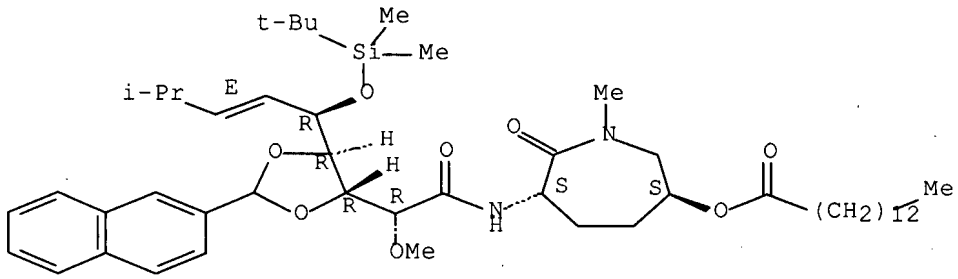
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



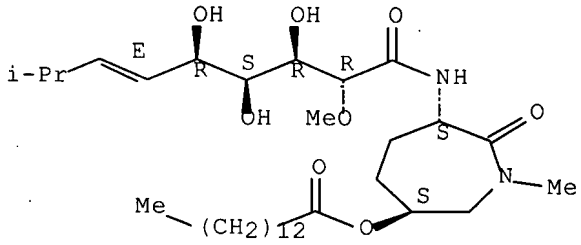
RN 547742-46-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,4-O-(2-naphthalenylmethylene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



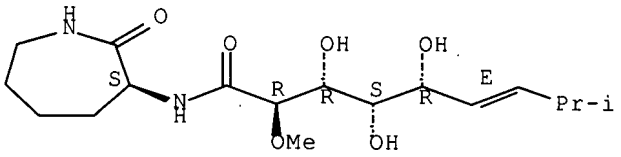
IT 104947-69-5P, Bengamide b 118477-03-5P
118477-10-4P, Bengamide z 442913-29-3P
442913-35-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(convergent and efficient enantioselective synthesis of bengamides via polyol intermediate)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



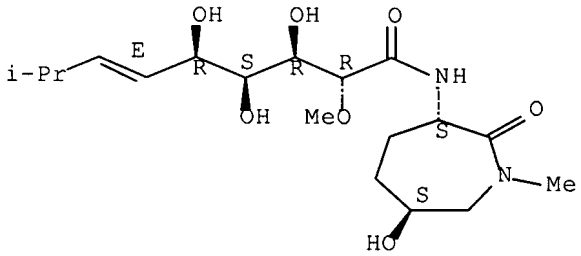
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



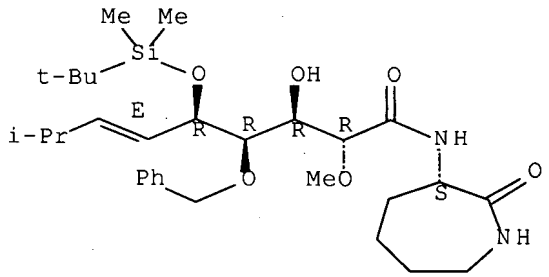
RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



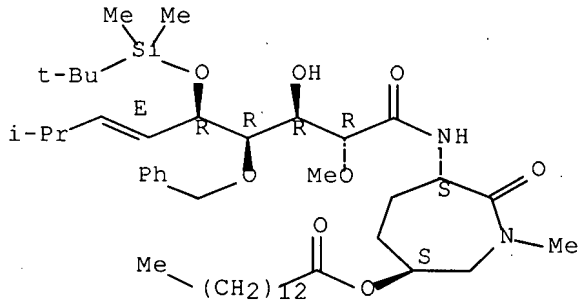
RN 442913-29-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



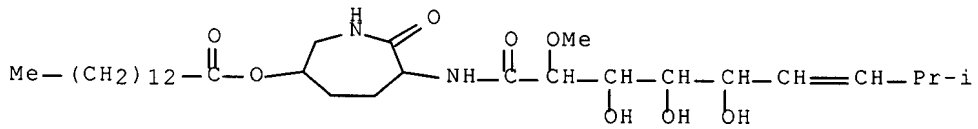
RN 442913-35-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



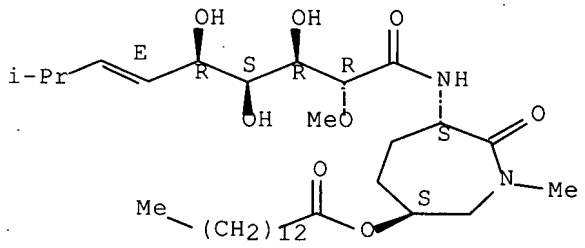
RE.CNT 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:4658 CAPLUS Full-text
DN 138:338418
TI Synthetic approaches toward the bengamide family of antitumor marine natural products. A review
AU Kinder, Frederick R., Jr.
CS Oncology Department, Novartis Pharmaceuticals Corporation, Summit, NJ, 07901-1398, USA
SO Organic Preparations and Procedures International (2002), 34(6), 559,561-583
CODEN: OPPIAK; ISSN: 0030-4948
PB Organic Preparations and Procedures, Inc.
DT Journal; General Review
LA English
AB A review. The bengamide class of sponge-derived natural products has been studied for over 15 yr. Antitumor bengamides are potent antiproliferative agents against both transformed and non-transformed cells. Future biol. profiling of bengamides depends on a reliable source of gram amts. of these compds. Harvesting bengamide-producing sponges or finding a bengamide-producing organism that could be grown in culture is most likely not feasible. This has led to a great deal of interest in producing suitable amts. of these compds. by total synthesis. In addition, a feasible synthesis would make the synthesis of analogs possible. All of the published bengamide syntheses from simple starting materials are reviewed in this work.
IT 104947-68-4P, Bengamide A 104947-69-5P, Bengamide B
118477-03-5P, Bengamide E 118477-04-6P, Bengamide F
118477-10-4P, Bengamide Z 331766-67-7P, Bengamide P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthetic approaches toward the bengamide family of antitumor marine natural products)
RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



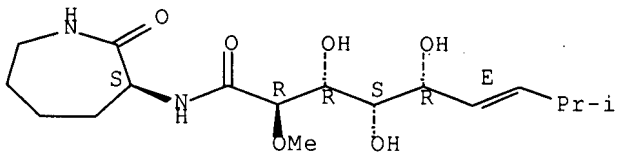
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

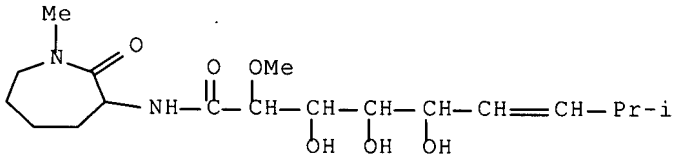


RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

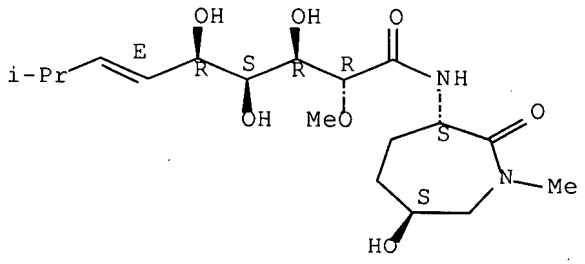


RN 118477-04-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



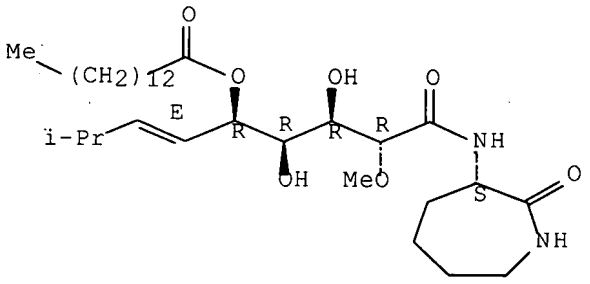
RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 331766-67-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-tetradecanoate, (6E)- (9CI) (CA INDEX NAME)

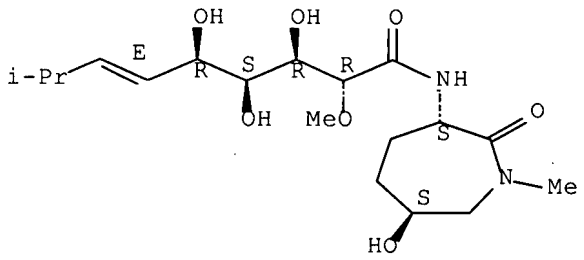
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:750153 CAPLUS Full-text
DN 137:278990
TI Part i. total synthesis of bengamide z. part ii. studies toward asymmetric acylation of alpha-oxygenated imides
AU Clark, Tammy Jo
CS Univ. of Rochester, Rochester, NY, USA
SO (2001) 225 pp. Avail.: UMI, Order No. DA3035598
From: Diss. Abstr. Int., B 2002, 62(12), 5730
DT Dissertation
LA English
AB Unavailable
IT 118477-10-4P, Bengamide Z
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of bengamide Z)
RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L10 ANSWER 18 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:696698 CAPLUS Full-text
DN 137:216888
TI Process for preparing certain substituted caprolactams
IN Xu, David Daqiang; Liu, Wenming
PA USA
SO U.S. Pat. Appl. Publ., 6 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002128474	A1	20020912	US 2002-95325	20020311
	US 6545148	B2	20030408		
	WO 2002072555	A1	20020919	WO 2002-EP2664	20020311
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VN, YU, ZA, ZW				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	AU 2002302411	A1	20020924	AU 2002-302411	20020311
PRAI	US 2001-275099P	P	20010312		
	WO 2002-EP2664	W	20020311		

OS CASREACT 137:216888; MARPAT 137:216888
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

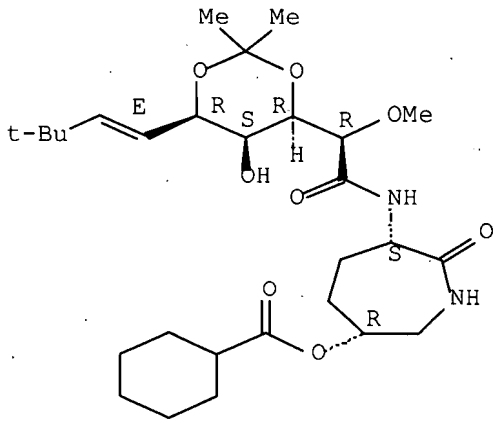
AB A process for the preparation of I [R1 = (cyclo)alkyl; R2 = H, alkyl; X = alkylene; alkenylene; alkynylene; m = 0-1;, R3 = cycloalkyl, (un)substituted Ph, furanyl, benzofuranyl, thiophenyl, etc.] was disclosed. Deprotection of (3S,6R)-3-((tert-butoxycarbonyl)amino)hexahydr o-6-(((cyclohexane)carbonyl)oxy)-2H-azepin-2-one (prior art; EtOAc/HCl, room temperature) and acylation of the resulting amine•HCl in the presence of sodium 2-ethylhexanoate and THF with II (prior art) at room temperature for 20 h provided an intermediate which upon treatment with TFA/THF at 0° for 30 min yielded III. The current process is milder than prior art methods.

IT 270902-71-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for preparing certain substituted caprolactams)

RN 270902-71-1 CAPLUS

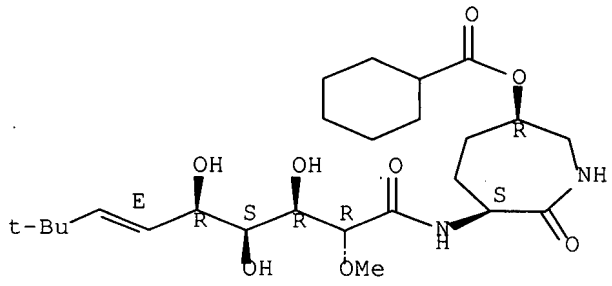
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



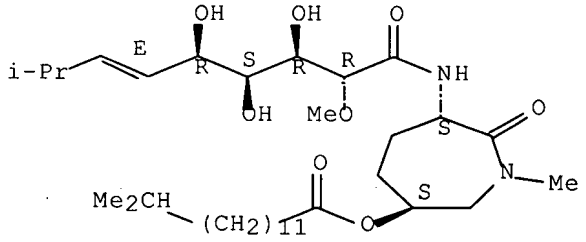
IT 270902-51-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for preparing certain substituted caprolactams)
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



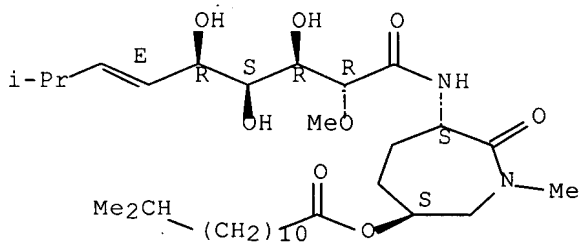
L10 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:695379 CAPLUS Full-text
DN 138:52906
TI Chemical investigation of biologically active marine natural products
AU Thale, Zia Irene
CS Univ. of California, Santa Cruz, CA, USA
SO (2001) 304 pp. Avail.: UMI, Order No. DA3032272
From: Diss. Abstr. Int., B 2002, 62(11), 5131
DT Dissertation
LA English
AB Unavailable
IT 331765-19-6P, Bengamide M 331766-12-2P, Bengamide O
331766-63-3P, Bengamide Q 331766-64-4P, Bengamide R
331766-65-5P, Bengamide N 331766-67-7P, Bengamide P
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation, mol. structure and cytotoxicity of biol. active marine natural products)
RN 331765-19-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-6-[(13-methyl-1-oxotetradecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



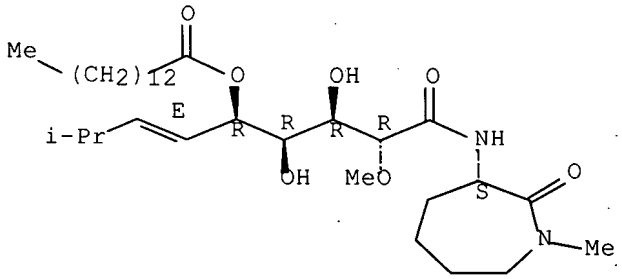
RN 331766-12-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-6-[(12-methyl-1-oxotridecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



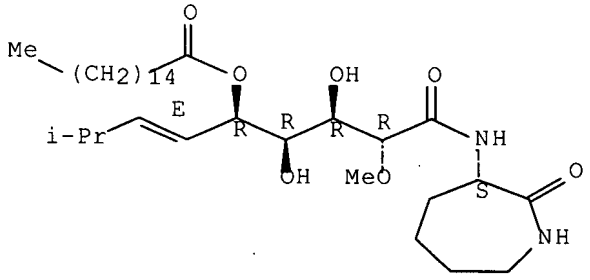
RN 331766-63-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-tetradecanoate, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



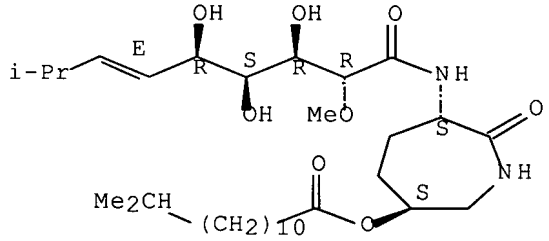
RN 331766-64-4 CAPLUS.
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-hexadecanoate, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



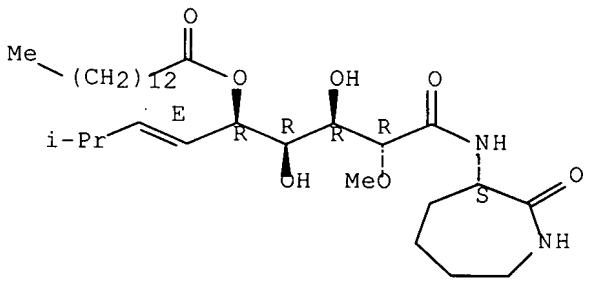
RN 331766-65-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-[(12-methyl-1-oxotridecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 331766-67-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-tetradecanoate, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.


Me
(CH2)12
O
O
OH
O
E
i-Pr
R
R
R
R
NH
OH
MeO
S
O
NH

L10 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:391505 CAPLUS Full-text
DN 136:380089
TI Method for screening methionine aminopeptidase inhibitory anti-proliferative compounds and method for inhibiting tumor growth
IN Phillips, Penny Elisabeth; Schindler, Patrick Andre; Towbin, Harry
PA Novartis Ag, Switz.; Novartis-Erfindungen Verwaltungsgesellschaft mbH; Novartis Pharma GmbH
SO PCT Int. Appl., 13 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

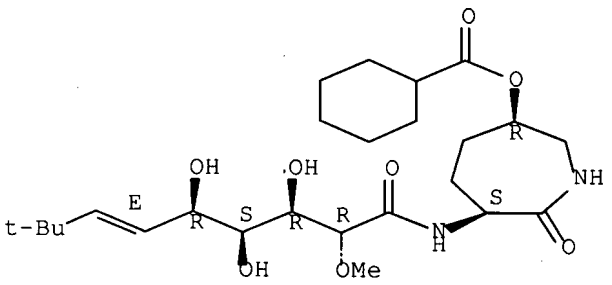
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002039990	A2	20020523	WO 2001-EP13076	20011112
	WO 2002039990	A3	20030313		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	AU 2002017020	A5	20020527	AU 2002-17020	20011112
	EP 1337854	A2	20030827	EP 2001-996369	20011112
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004514122	T	20040513	JP 2002-542365	20011112
	US 2004048318	A1	20040311	US 2003-416669	20030903
PRAI	US 2000-248489P	P	20001114		
	WO 2001-EP13076	W	20011112		

AB The invention discloses a method for evaluating the antiproliferative activity of compds. having MetAP inhibitory activity, as well as a method for screening compds. that inhibit angiogenesis or growth of tumors. The invention addnl. provides a method for monitoring the progress of treatment for controlling angiogenesis or the growth of tumors.

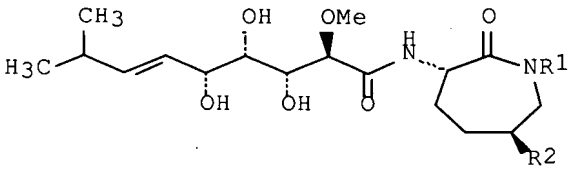
IT 270902-51-7, LAF 389
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methionine aminopeptidase inhibitory anti-proliferative compound screening, and method for inhibiting tumor growth)

RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

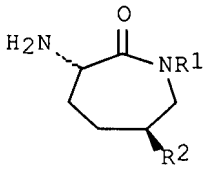
Absolute stereochemistry.
Double bond geometry as shown.


O
O
R
NH
OH
OH
O
E
S
S
t-Bu
R
R
R
N
H
O
OH
OMe

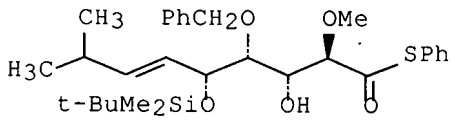
L10 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:372447 CAPLUS Full-text
DN 137:109460
TI A Practical Enantioselective Total Synthesis of the Bengamides B, E, and Z
AU Boeckman, Robert K., Jr.; Clark, Tammy J.; Shook, Brian C.
CS Department of Chemistry, University of Rochester, Rochester, NY, 14627-0216, USA
SO Organic Letters (2002), 4(12), 2109-2112
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 137:109460
GI



I



III



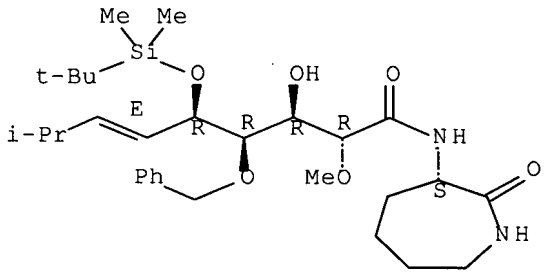
II

AB A practical total synthesis of bengamides Z, B and E, I [R1 = Me, R2 = OH; R1 = Me, R2 = O2C(CH2)12Me; R1 = R2 = H, resp.], via a protected polyol II intermediate, obtained from consecutive aldol condensations, was accomplished. Chiral phase transfer-catalyzed enantioselective alkylation afforded the more highly functionalized aminocaprolactams III [R1 = Me, R2 = OAc; R1 = Me, R2 = O2C(CH2)12Me] required for Bengamides Z and B. 2-Naphthylmethyl ether protecting group, compatible with the boron Lewis acids required for enantioselective aldol condensation, was utilized in the synthesis of Bengamide B.

IT 442913-29-3P 442913-34-0P 442913-35-1P
442913-40-8P 442913-43-1P 442913-44-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. total synthesis of bengamides B, E and Z using protected, polyol intermediates and substituted aminocaprolactams)

RN 442913-29-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

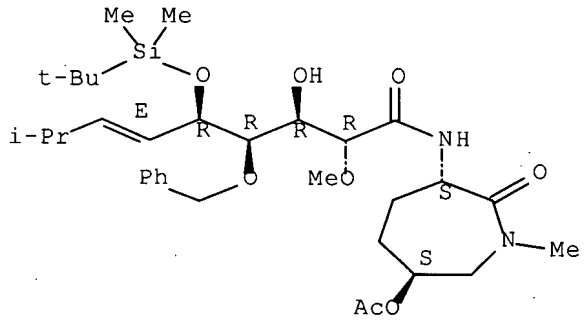
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 442913-34-0 CAPLUS

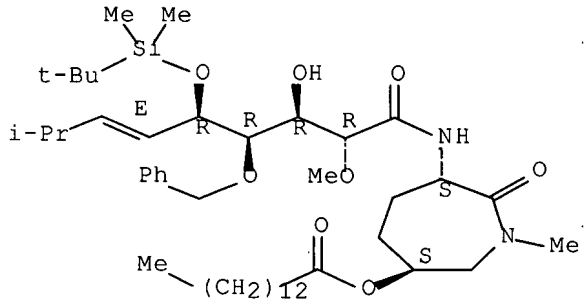
CN D-gulo-Non-6-enonamide, N-[(3S,6S)-6-(acetyloxy)hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



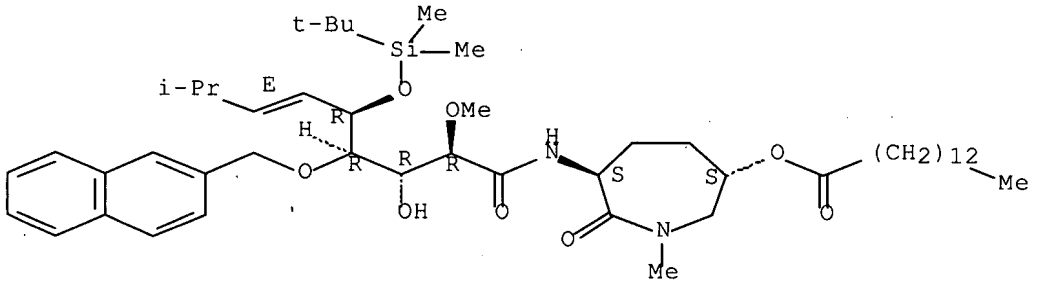
RN 442913-35-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



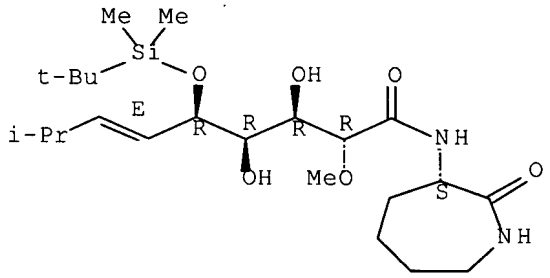
RN 442913-40-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(2-naphthalenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



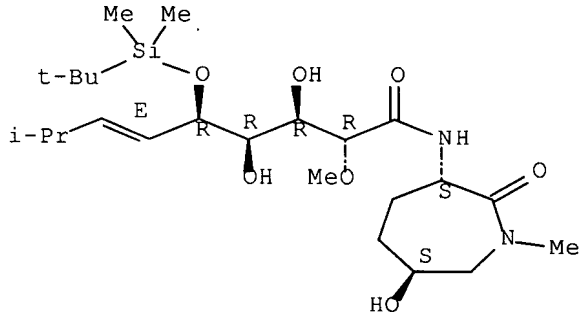
RN 442913-43-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



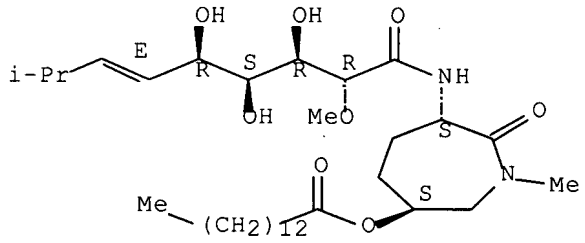
RN 442913-44-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



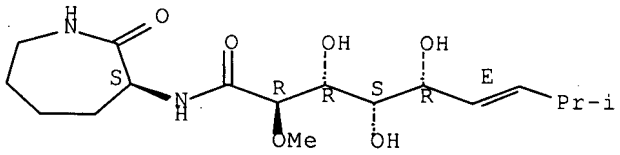
IT 104947-69-5P 118477-03-5P 118477-10-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. total synthesis of bengamides B, E and Z using protected, polyol intermediates and substituted aminocaprolactams)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

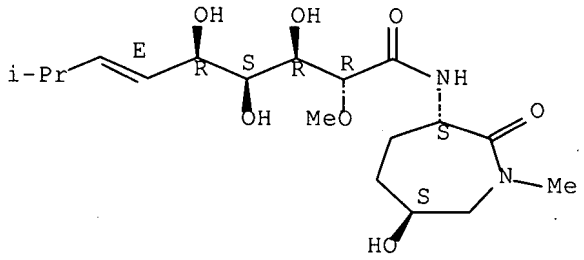
Absolute stereochemistry.
Double bond geometry as shown.



RN 118477-10-4 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

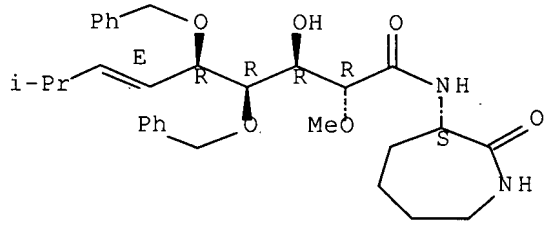
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

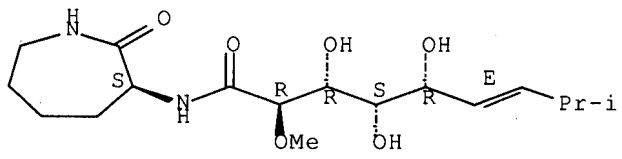
L10 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:97953 CAPLUS Full-text
DN 136:401986
TI Total synthesis of bengamide E
AU Liu, Wenming; Szewczyk, Joanna M.; Waykole, Liladhar; Repic, Oljan; Blacklock, Thomas J.
CS Chemical and Analytical Development, Process R&D, Novartis Institute for Biomedical Research, East Hanover, NJ, 07936, USA
SO Tetrahedron Letters (2002), 43(8), 1373-1375
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 136:401986
AB A total synthesis of bengamide E is reported. The synthesis includes the utilization of (2S,3S)-tartrate as the chiral building block, construction of the E-olefin by the Julia protocol, an aldol reaction to generate C-2 and C-3 centers with anti stereochem., and coupling of the thioester with caprolactam hydrochloride using sodium 2-ethylhexanoate.
IT 430473-73-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)(total synthesis of bengamide E from D-tartrate as the chiral building block)
RN 430473-73-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4,5-bis-O-(phenylmethyl)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of bengamide E from D-tartrate as the chiral building block)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

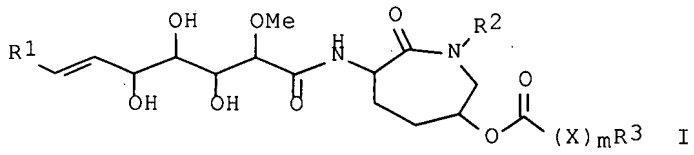


RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:851792 CAPLUS Full-text
DN 135:366736
TI Preparation and use of substituted caprolactams in treating tumors
IN Kinder, Frederick Ray, Jr.; Bair, Kenneth Walter; Jagoe, Christopher Turchik; Versace, Richard William; Wattanasin, Sompong
PA Novartis AG, Switz.
SO U.S. Pat. Appl. Publ., 21 pp., Cont.-in-part of Ser. No. US 1999-441739, filed on 17 Nov 1999, now patentedPa
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2001044433	A1	20011122	US 2001-805010	20010312
	US 6555533	B2	20030429		
	US 6239127	B1	20010529	US 1999-441739	19991117
PRAI	US 1998-172254P	P	19981117		
	US 1999-441739	A2	19991117		

OS CASREACT 135:366736; MARPAT 135:366736
GI



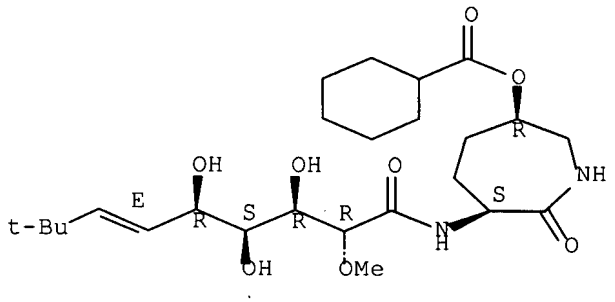
I

AB The invention provides substituted caprolactam compds. I (R1 = C1-6 alkyl, C3-6 cycloalkyl; R2 = H, C1-6 alkyl; X = C1-12 alkylene, C2-12 alkenylene, C2-12 alkynylene; m = 0, 1; R3 = C3-8 cycloalkyl, aromatic ring), pharmaceutical compns. containing the compds., the use of the compds. in treating tumors, and a process for making the compds.

IT 270902-51-7P 270902-52-8P 270902-53-9P
270902-54-0P 270902-55-1P 270902-56-2P
270902-57-3P 270902-58-4P 270902-59-5P
270902-61-9P 270902-62-0P 270902-63-1P
270902-64-2P 373354-14-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(caprolactam derivative preparation and use in treating tumors)

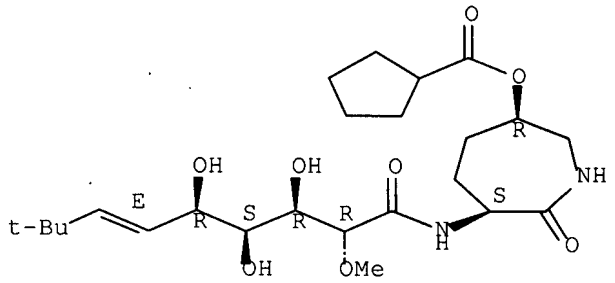
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



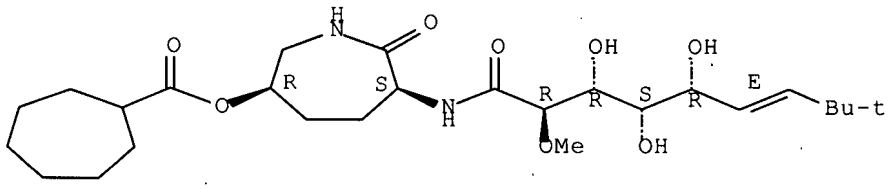
RN 270902-52-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclopentylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-53-9 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cycloheptylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

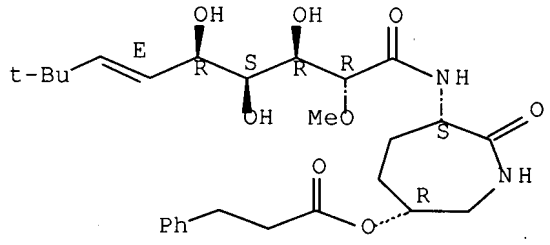
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-54-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-(1-oxo-3-phenylpropoxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

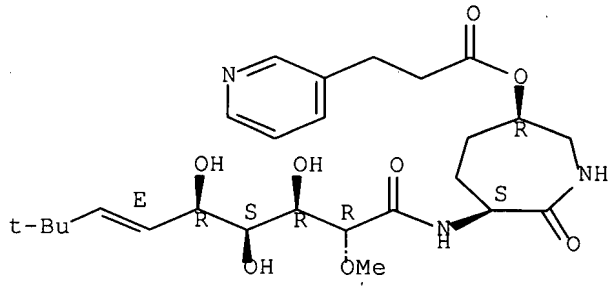
Absolute stereochemistry.

Double bond geometry as shown.



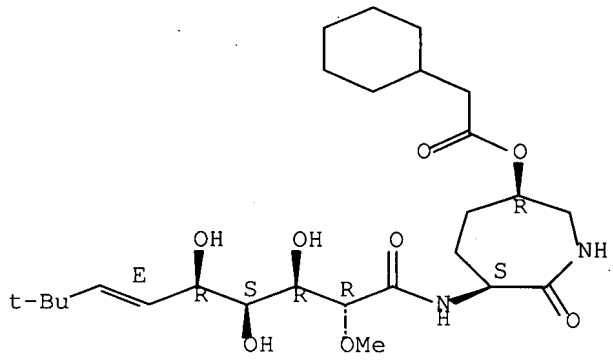
RN 270902-55-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[1-oxo-3-(3-pyridinyl)propoxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



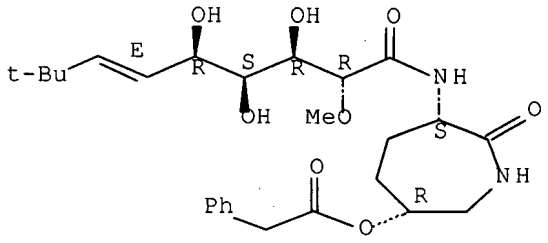
RN 270902-56-2 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylacetyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



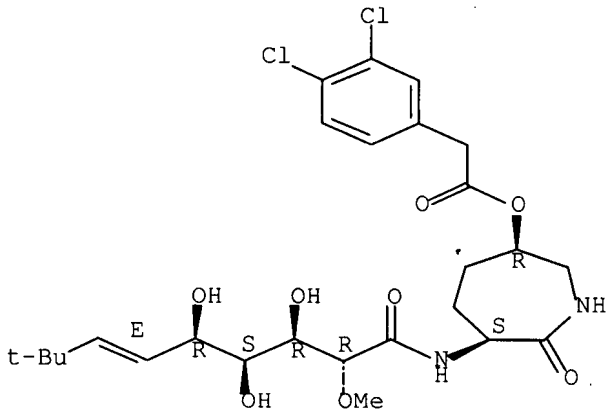
RN 270902-57-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(phenylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



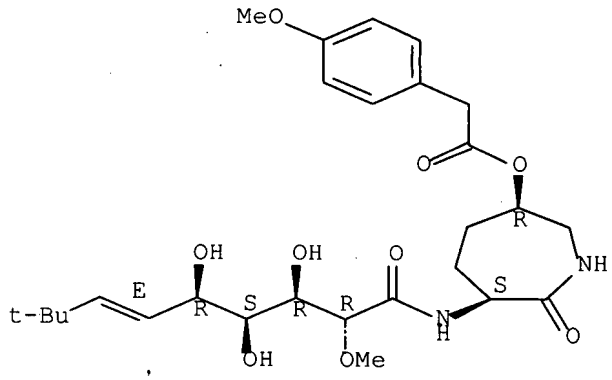
RN 270902-58-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(3,4-dichlorophenyl)acetyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



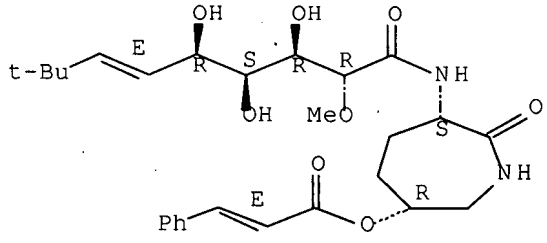
RN 270902-59-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[[(4-methoxyphenyl)acetyl]oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



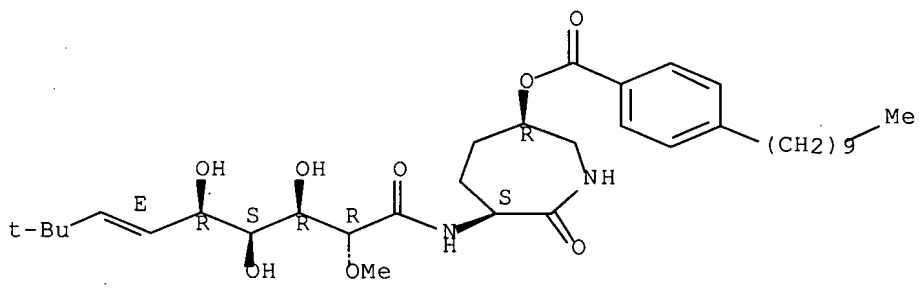
RN 270902-61-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-62-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(4-decylbenzoyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

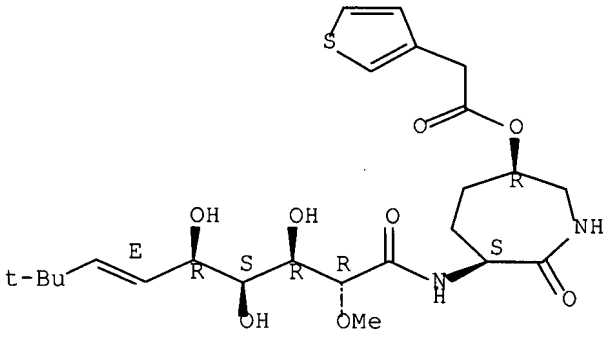
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-63-1 CAPLUS

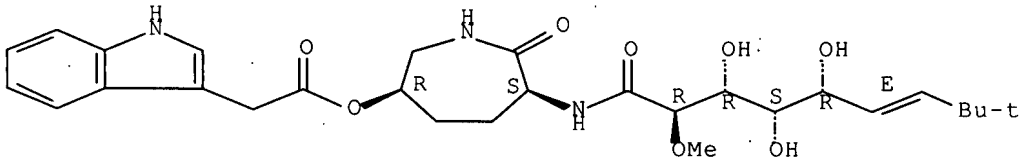
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(3-thienylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



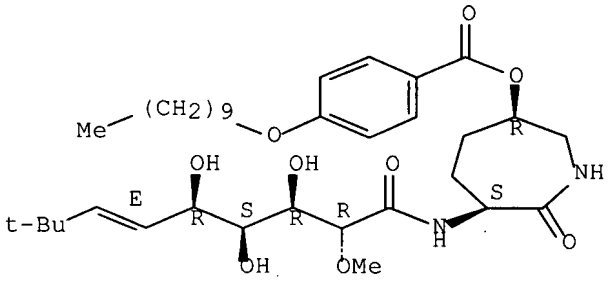
RN 270902-64-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[(1H-indol-3-ylacetyl)oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



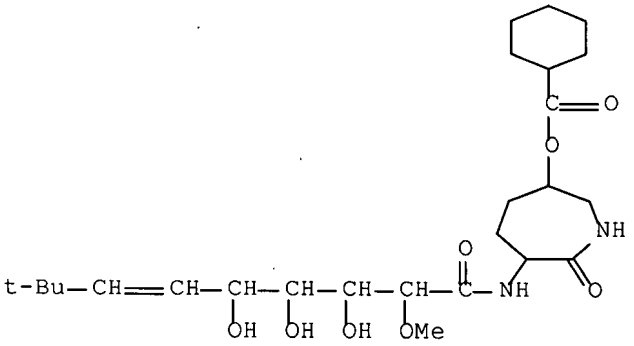
RN 373354-14-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[4-(decyloxy)benzoyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

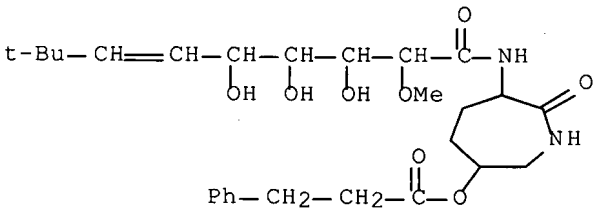


IT 374602-77-4 374602-78-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(caprolactam derivative preparation and use in treating tumors)

RN 374602-77-4 CAPLUS
CN Non-6-enonamide, N-[6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



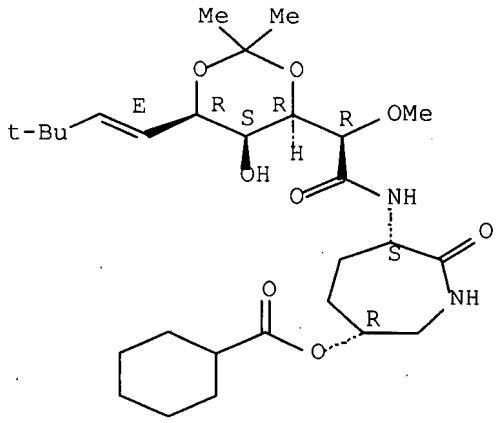
RN 374602-78-5 CAPLUS
CN Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-(1-oxo-3-phenylpropoxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



IT 270902-71-1P 270902-74-4P 270902-75-5P
270902-76-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction; caprolactam derivative preparation and use in treating
tumors)

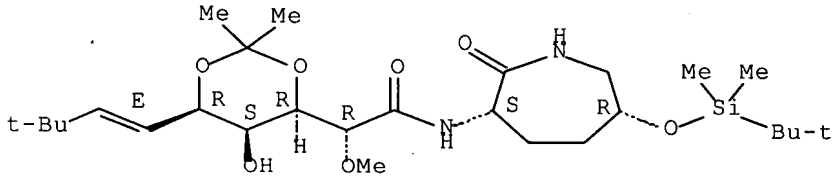
RN 270902-71-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



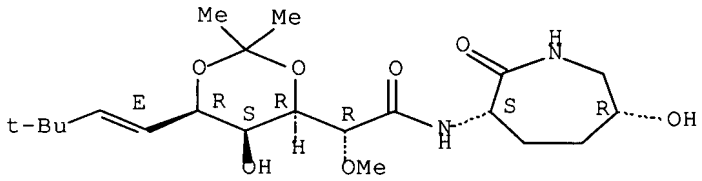
RN 270902-74-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



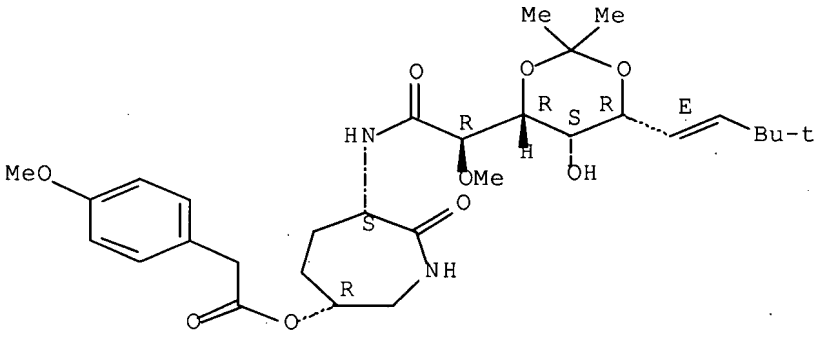
RN 270902-75-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



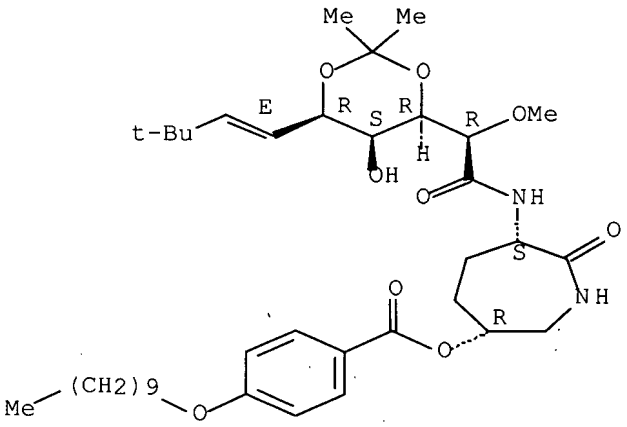
RN 270902-76-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[[(4-methoxyphenyl)acetyl]oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



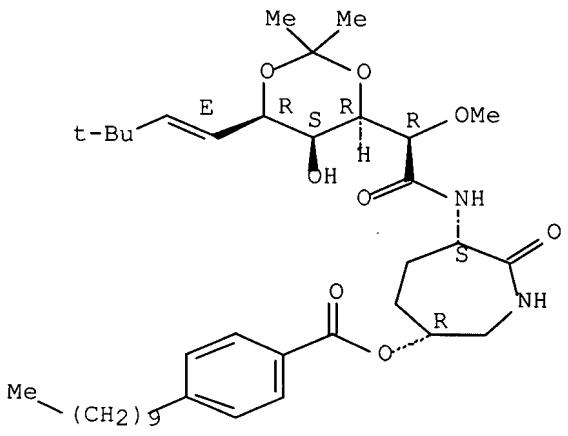
IT 374602-87-6P 374602-89-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction; caprolactam derivative preparation and use in treating tumors)
RN 374602-87-6 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[4-(decyloxy)benzoyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 374602-89-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(4-decylbenzoyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.


Me
Me
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E
R
S
R
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OMe
t-Bu
OH
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NH
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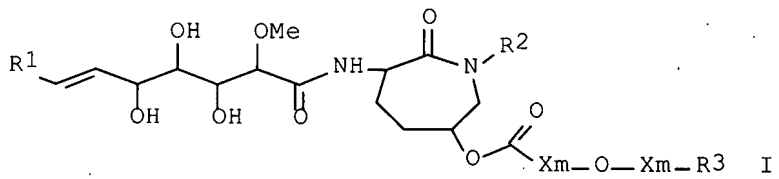
(CH2)9

L10 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:833287 CAPLUS Full-text
DN 135:357854
TI Preparation of substituted caprolactam carbonates and ethers and their use as antitumor agents
IN Kinder, Frederick Ray, Jr.; Versace, Richard William; Bair, Kenneth Walter
PA Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft M.B.H.
SO PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001085697	A1	20011115	WO 2001-EP5263	20010509
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6413954	B1	20020702	US 2001-850852	20010508
	CA 2405892	A1	20011115	CA 2001-2405892	20010509
	EP 1282604	A1	20030212	EP 2001-975824	20010509
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2001010641	A	20030318	BR 2001-10641	20010509
	JP 2003532711	T	20031105	JP 2001-582298	20010509
	US 2003055041	A1	20030320	US 2002-150778	20020517
	US 6599898	B2	20030729		
PRAI	US 2000-325753P	P	20000511		
	US 2000-568667	A	20000511		
	US 2001-850852	A3	20010508		
	WO 2001-EP5263	W	20010509		

OS MARPAT 135:357854
GI



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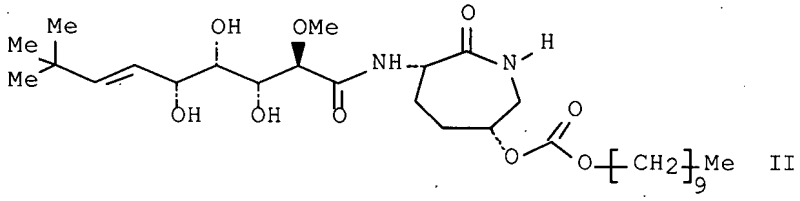


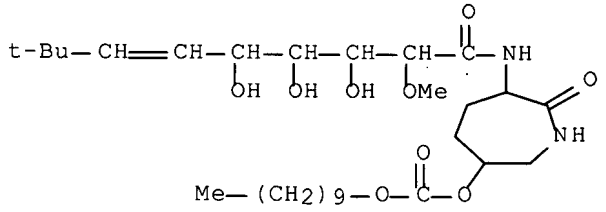
II

AB Substituted caprolactam carbonate and ether compds. of following formula I wherein R1 is alkyl, cycloalkyl; R2 is H, alkyl; each X is independently alkylene; m is 0, 1; R3 is alkyl, alkenyl, cycloalkyl, substituted aromatic ring, were prepared as antitumor agents. Thus, caprolactam carbonate II was prepared and tested in nude mouse as a model to inhibit the growth of human tumor xenografts in a typical i.v. dosage of 20 mg/kg, three to five times a week as antitumor agent (EC50 = 0.21 ± 0.14 μM).

IT 372165-59-8P 372165-60-1P 372165-61-2P
372165-62-3P 372165-63-4P 372165-64-5P
372165-65-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claim compound; preparation of substituted caprolactam carbonates and ethers
and their use as antitumor agents)

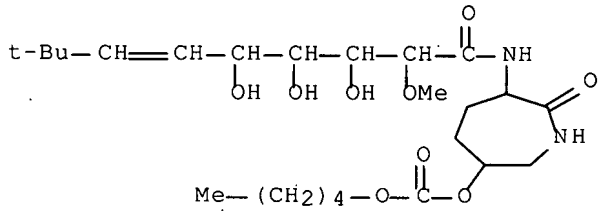
RN 372165-59-8 CAPLUS

CN Non-6-enonamide, N-[6-[[(decyloxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



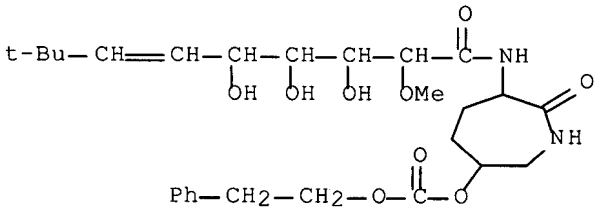
RN 372165-60-1 CAPLUS

CN Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[[(pentyloxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)

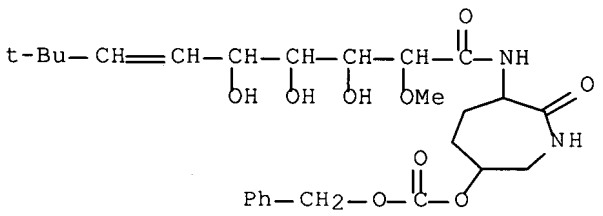


RN 372165-61-2 CAPLUS

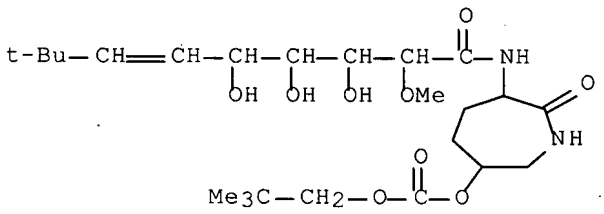
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[[(2-phenylethoxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



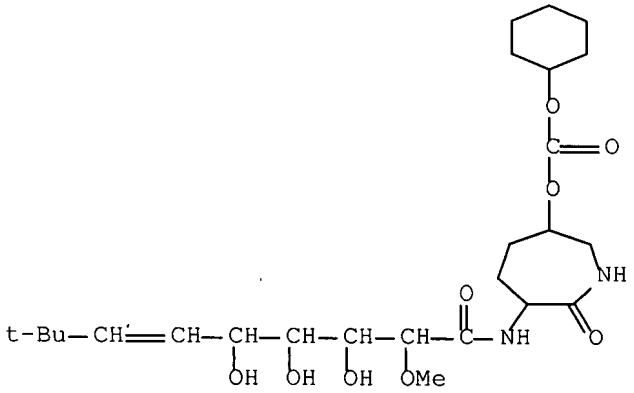
RN 372165-62-3 CAPLUS
CN Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[[(phenylmethoxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



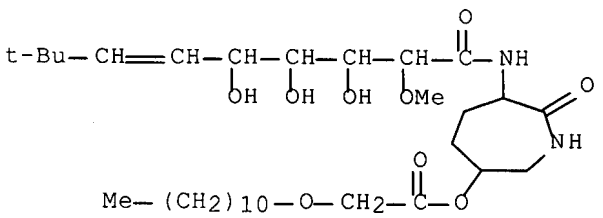
RN 372165-63-4 CAPLUS
CN Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[6-[[(2,2-dimethylpropoxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



RN 372165-64-5 CAPLUS
CN Non-6-enonamide, N-[6-[[(cyclohexyloxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)

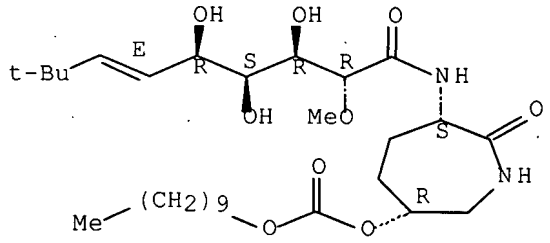


RN 372165-65-6 CAPLUS
CN Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[[(undecyloxy)acetyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl- (9CI) (CA INDEX NAME)



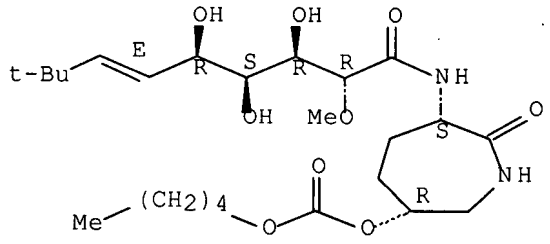
IT 372165-47-4P 372165-48-5P 372165-49-6P
372165-50-9P 372165-51-0P 372165-52-1P
372165-53-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted caprolactam carbonates and ethers and their use as antitumor agents)
RN 372165-47-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[(decyloxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



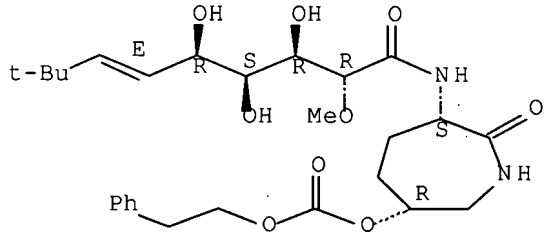
RN 372165-48-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(pentyloxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 372165-49-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(2-phenylethoxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

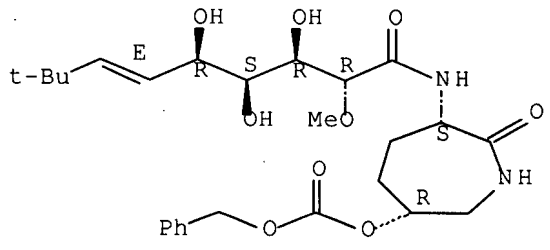
Absolute stereochemistry.
Double bond geometry as shown.



RN 372165-50-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(phenylmethoxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

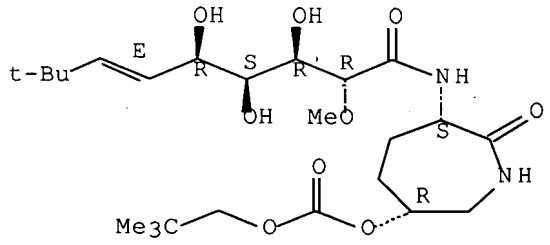
Absolute stereochemistry.

Double bond geometry as shown.



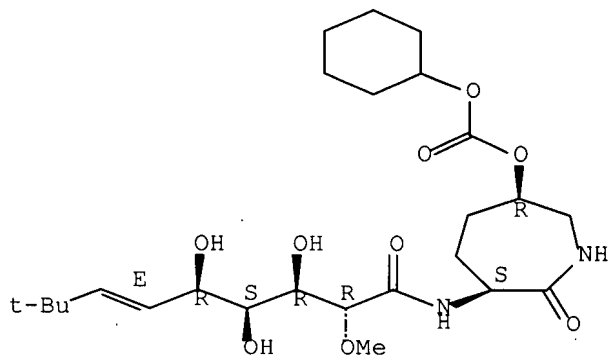
RN 372165-51-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(2,2-dimethylpropoxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



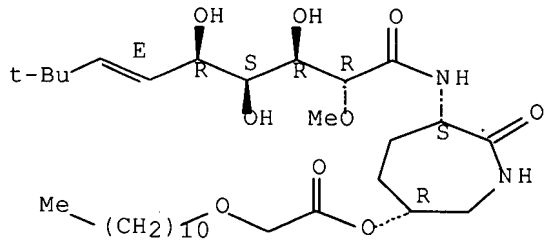
RN 372165-52-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[(cyclohexyloxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 372165-53-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(undecyloxy)acetyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

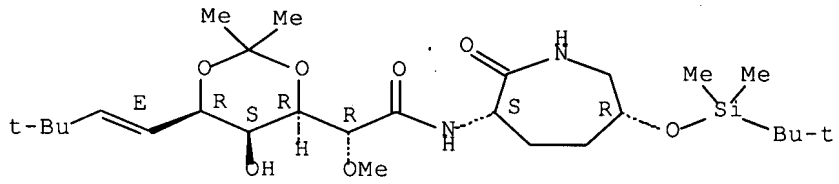
Absolute stereochemistry.
Double bond geometry as shown.



IT 270902-74-4P 270902-75-5P 372165-54-3P
372165-57-6P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted caprolactam carbonates and ethers and their use as antitumor agents)

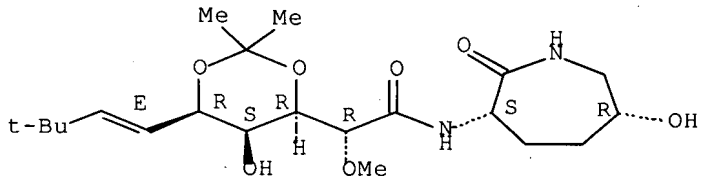
RN 270902-74-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



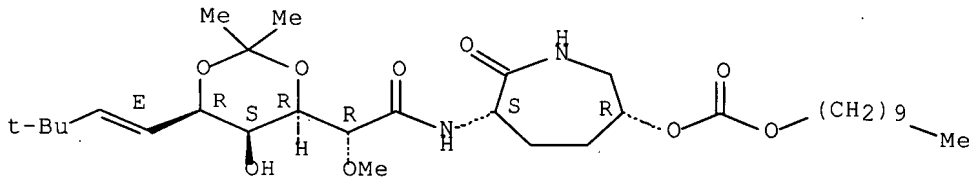
RN 270902-75-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



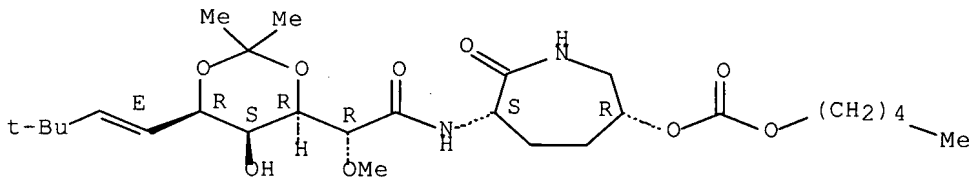
RN 372165-54-3 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[(decyloxy)carbonyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



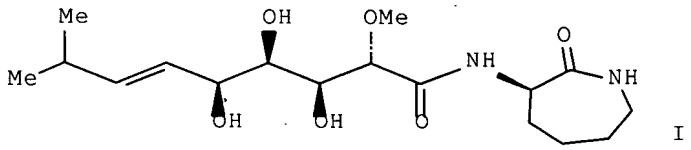
RN 372165-57-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(pentyloxy)carbonyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:667418 CAPLUS Full-text
DN 135:358127
TI A Chemoenzymatic Total Synthesis of ent-Bengamide E
AU Banwell, Martin G.; McRae, Kenneth J.
CS Research School of Chemistry Institute of Advanced Studies, The Australian National University, Canberra, 0200, Australia
SO Journal of Organic Chemistry (2001), 66(20), 6768-6774
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 135:358127
GI



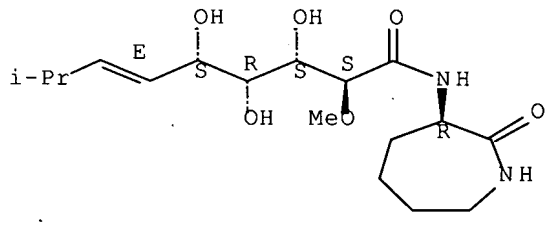
I

AB The cis-1,2-dihydrocatechol, which can be obtained in enantiomerically pure form by microbial dihydroxylation of bromobenzene, has been converted into the enantiomer (I) of the cyclolysine-based marine natural product bengamide E.

IT 372961-78-9P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(chemoenzymic total synthesis and antitumor activity of ent-bengamide E)

RN 372961-78-9 CAPLUS
CN L-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3R)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

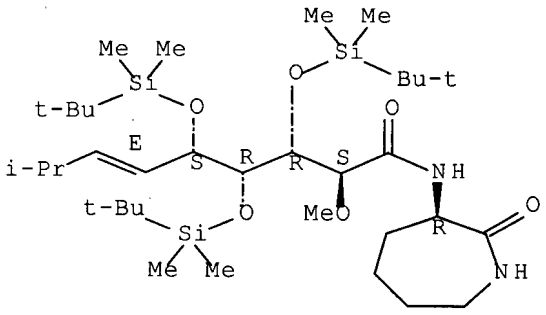


IT 373388-68-2P
RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(chemoenzymic total synthesis and antitumor activity of ent-bengamide E)

RN 373388-68-2 CAPLUS
CN L-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-3,4,5-tris-O-[(1,1-

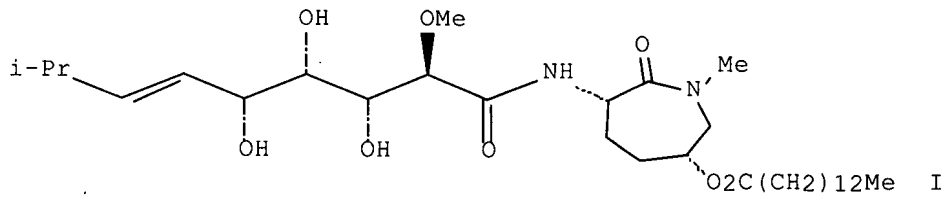
dimethylethyl)dimethylsilyl]-N-[(3R)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

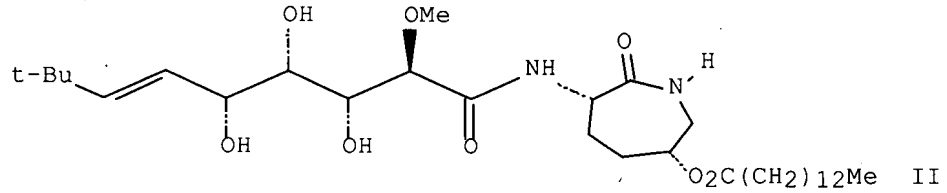


RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:667282 CAPLUS Full-text
DN 135:371966
TI Synthesis and Antitumor Activity of Ester-Modified Analogues of Bengamide B
AU Kinder, Frederick R., Jr.; Versace, Richard W.; Bair, Kenneth W.; Bontempo, John M.; Cesarz, David; Chen, Steven; Crews, Phillip; Czuchta, Ania M.; Jagoe, Christopher T.; Mou, Yin; Nemzek, Raphael; Phillips, Penny E.; Tran, Long D.; Wang, RunMing; Weltchek, Susan; Zabludoff, Sonya
CS Oncology Department, Novartis Pharmaceuticals Corporation, Summit, NJ, 07901-1398, USA
SO Journal of Medicinal Chemistry (2001), 44(22), 3692-3699
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 135:371966
GI



I



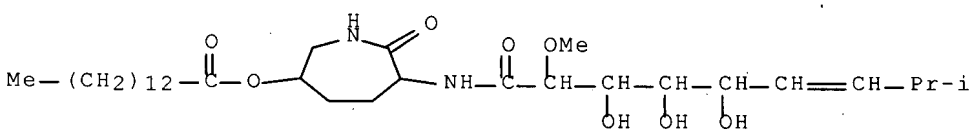
II

AB Bengamide B (I), a novel sponge-derived marine natural product with broad spectrum antitumor activity, was not suitable for further preclin. development because of its difficult synthesis and very poor water solubility I produced a 31% T/C at its solubility-limited maximum i.v. dose of 33 μmol/kg in MDA-MB-435 breast carcinoma implanted s.c. as a xenograft in nude mice. Bengamide B analog (II) with three structural changes (t-Bu alkene substituent, unsubstituted lactam nitrogen, and inverted lactam 5'-myristoyloxy group), was as potent as I in vitro and more efficacious than I in vivo. A series of ester-modified analogs based on II were synthesized and tested in vitro and in vivo (MDA-MB-435). The cyclohexyl- and phenethyl-substituted esters, resp., had in vitro and in vivo activities similar to that of II and enhanced water solubility (ca. 1 mg/mL). Consequently, they were tested in the MDA-MB-435 xenograft model at 100 μmol/kg and produced 29% and 57% tumor regression, resp.
IT 104947-68-4, Bengamide A 104947-69-5, Bengamide B
118477-03-5, Bengamide E 118477-04-6, Bengamide F
118477-10-4, Bengamide Z 331766-67-7, Bengamide P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(synthesis and antitumor activity of ester-modified analogs of bengamide B)

RN 104947-68-4 CAPLUS

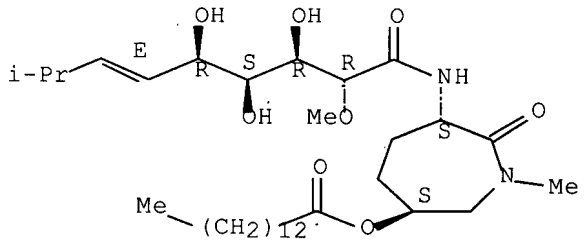
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



RN 104947-69-5 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

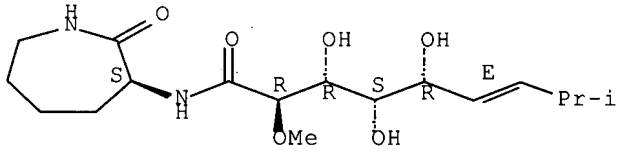
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 118477-03-5 CAPLUS

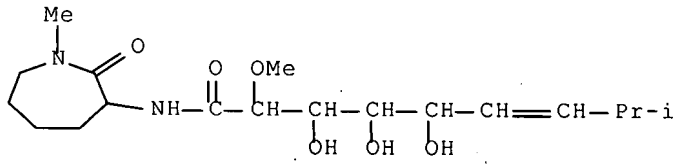
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



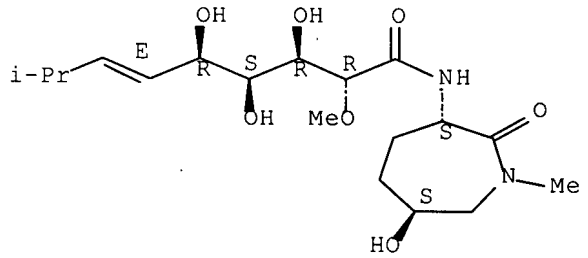
RN 118477-04-6 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



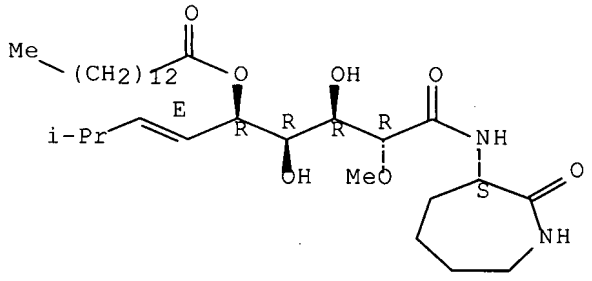
RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 331766-67-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-tetradecanoate, (6E)- (9CI) (CA INDEX NAME)

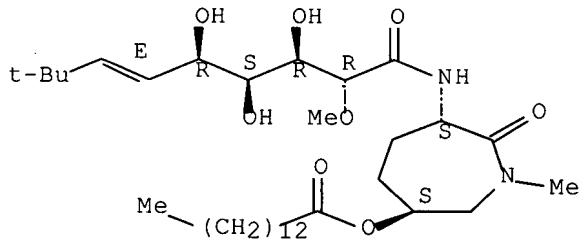
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 373354-08-6P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and antitumor activity of ester-modified analogs of bengamide B)
RN 373354-08-6 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

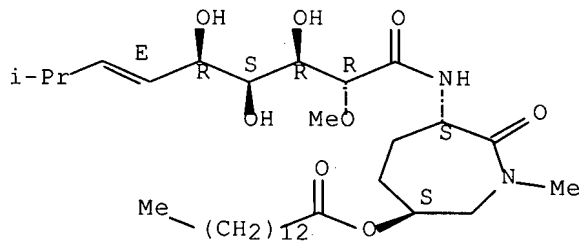
Absolute stereochemistry.
Double bond geometry as shown.



IT 104947-69-5DP, Bengamide B, derivs. 270902-51-7P 270902-52-8P 270902-53-9P 270902-54-0P 270902-55-1P 270902-56-2P 270902-57-3P 270902-61-9P 270902-62-0P 373354-09-7P 373354-11-1P 373354-12-2P 373354-13-3P 373354-14-4P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and antitumor activity of ester-modified analogs of bengamide B)

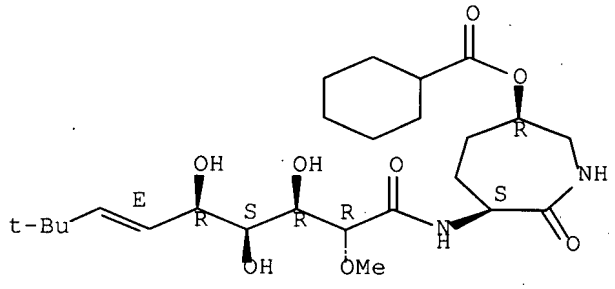
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



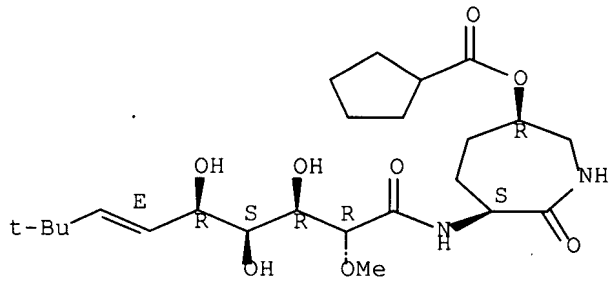
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



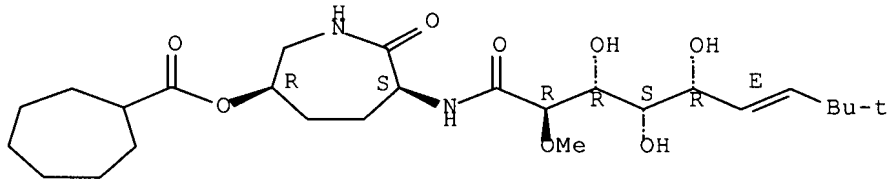
RN 270902-52-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclopentylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-53-9 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cycloheptylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

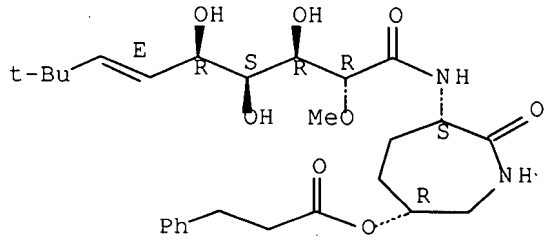
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-54-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-(1-oxo-3-phenylpropoxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

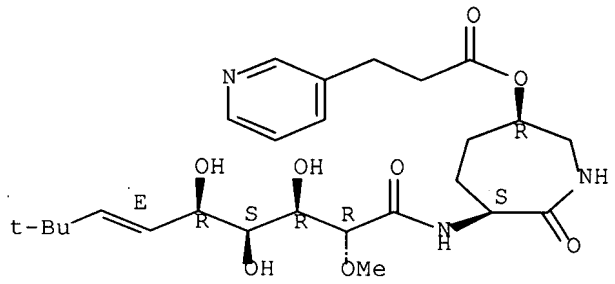
Absolute stereochemistry.

Double bond geometry as shown.



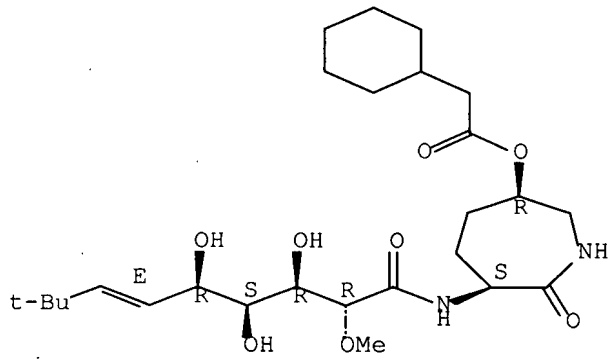
RN 270902-55-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[1-oxo-3-(3-pyridinyl)propoxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



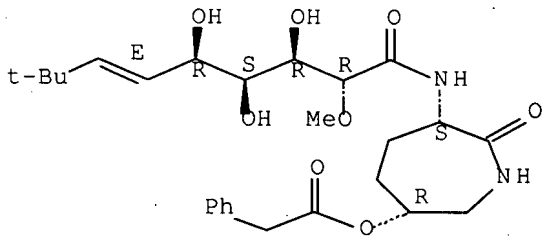
RN 270902-56-2 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylacetyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



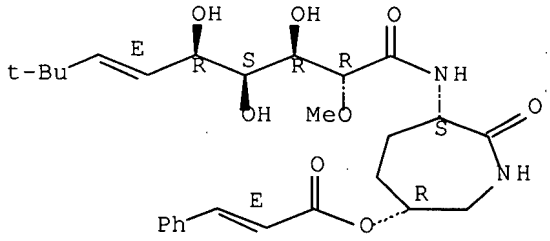
RN 270902-57-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(phenylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



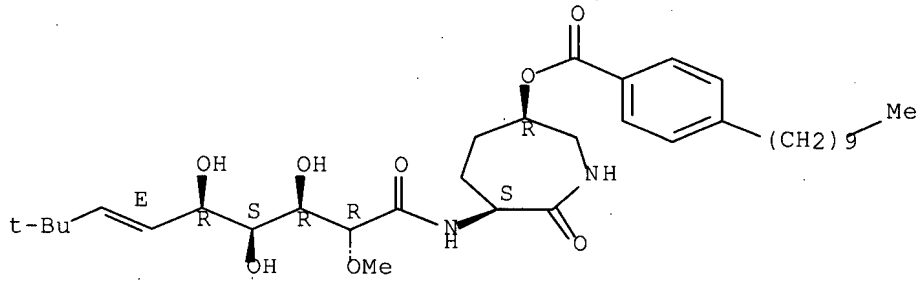
RN 270902-61-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



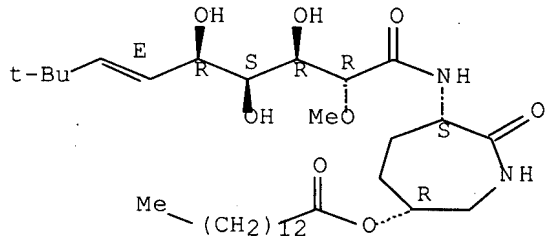
RN 270902-62-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(4-decylbenzoyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



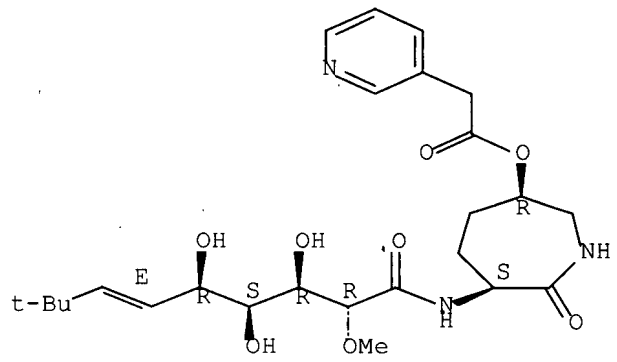
RN 373354-09-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 373354-11-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(3-pyridinylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

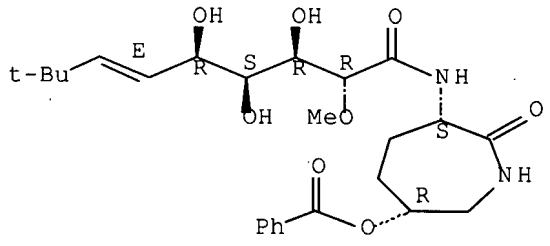
Absolute stereochemistry.
Double bond geometry as shown.



RN 373354-12-2 CAPLUS

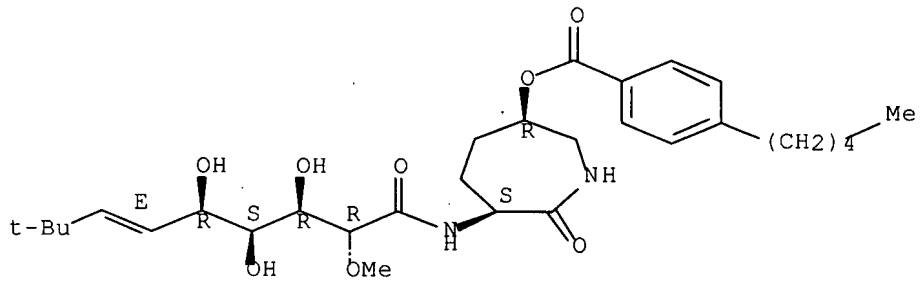
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-(benzoyloxy)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



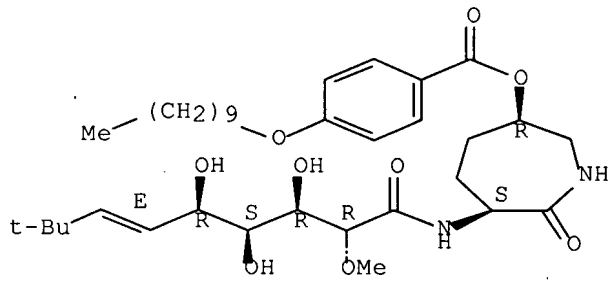
RN 373354-13-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(4-pentylbenzoyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 373354-14-4 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[4-(decyloxy)benzoyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

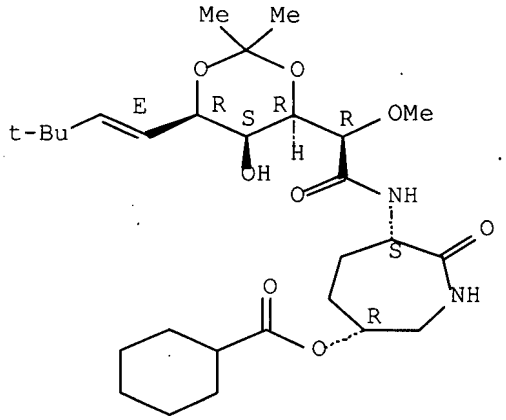
Absolute stereochemistry.
Double bond geometry as shown.



IT 270902-71-1P 270902-74-4P 270902-75-5P
373354-16-6P 373354-17-7P 373354-18-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and antitumor activity of ester-modified analogs of bengamide B)

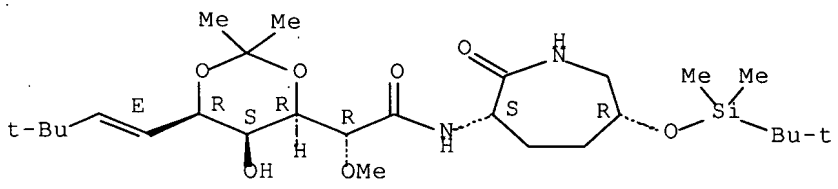
RN 270902-71-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 270902-74-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

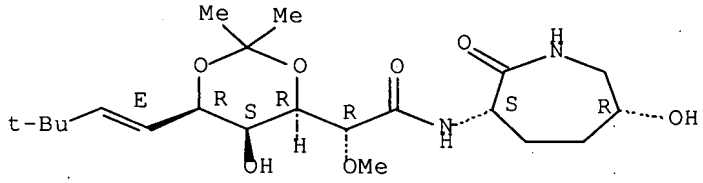
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-75-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

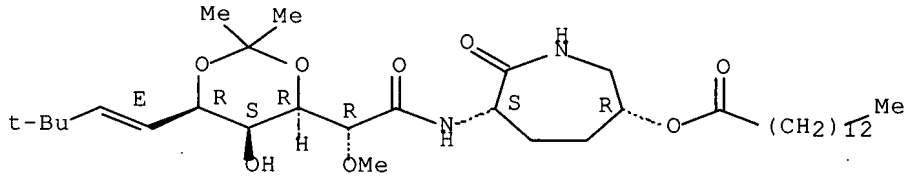
Absolute stereochemistry.

Double bond geometry as shown.



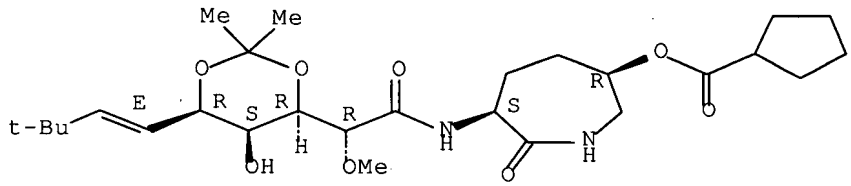
RN 373354-16-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



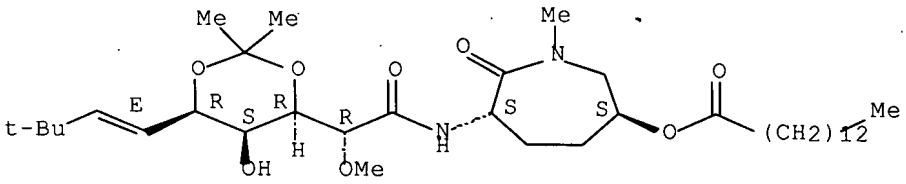
RN 373354-17-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclopentylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



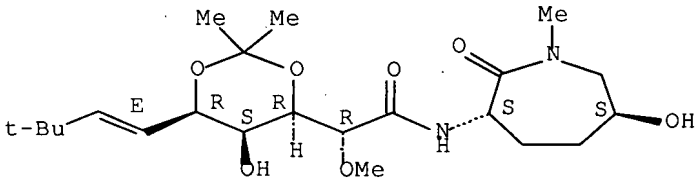
RN 373354-18-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 724452-96-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and antitumor activity of ester-modified analogs of bengamide B)
RN 724452-96-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:392061 CAPLUS Full-text
DN 135:5816
TI Preparation and use of substituted caprolactams as anticancer agents
IN Kinder, Frederick Ray, Jr.; Bair, Kenneth Walter; Jagoe, Christopher Turchik; Versace, Richard William; Wattanasin, Sompong
PA Novartis A.-G., Switz.
SO U.S., 18 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6239127	B1	20010529	US 1999-441739	19991117
	US 2001044433	A1	20011122	US 2001-805010	20010312
	US 6555533	B2	20030429		
PRAI	US 1998-172254P	P	19981117		
	US 1999-441739	A2	19991117		

OS CASREACT 135:5816; MARPAT 135:5816
GI

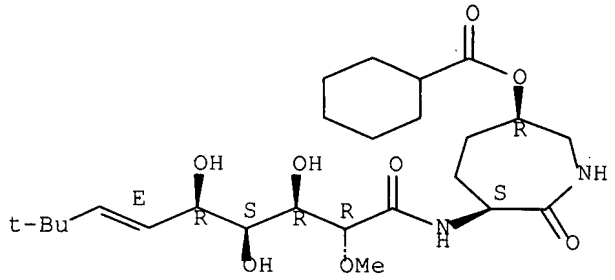
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Caprolactams I and their corresponding pharmaceutically acceptable addition salts were prepared and used as anti-tumor agents [wherein; R1 = (C1-6)alkyl or (C3-6)cycloalkyl; R2 = H or (C1-6)alkyl; X = (C1-12)alkylene, (C2-12)alkenylene; or (C2-12)alkynylene; n = 0 or 1; and R3 is (C3-8)cycloalkyl or an aromatic ring system selected from (un)substituted (Ph, (benzo)thiophene, pyrrole, indole or pyridine)]. Fourteen synthetic examples were provided. The process claimed is represented by the synthesis of III. Thus, (6E)-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl- 3,5-O-(1-methylethylidene)-gulo-non-6-enonic acid lactone II, prepared in 5 steps from α-D-glucopheptonic γ-lactone was treated with (3S,6R)-3-aminohexahydro-6-(cyclohexanecarbonyloxy)-2H-azepin-2-one to give the azepinylnonenamide III. The IC50 of III against MDA-MB-435 cells was 0.068 μM. Anti-tumor activity was also demonstrated by using the athymic nude mouse model (MDA-MB435 breast carcinoma); III gave a %T/C of -6% (6% reduction in tumor volume) at a dose of 100 μM/kg i.v. over 3 wk.

IT 270902-51-7P 270902-52-8P 270902-53-9P
270902-54-0P 270902-55-1P 270902-56-2P
270902-57-3P 270902-58-4P 270902-59-5P
270902-60-8P 270902-61-9P 270902-62-0P
270902-63-1P 270902-64-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of substituted caprolactams as antitumor agents)

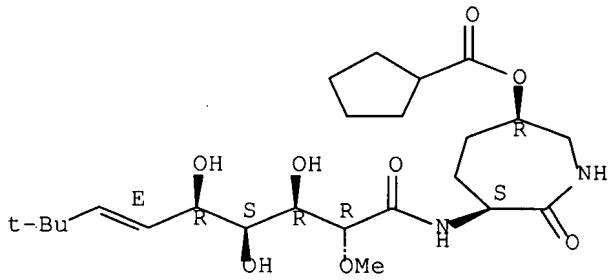
RN 270902-51-7 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



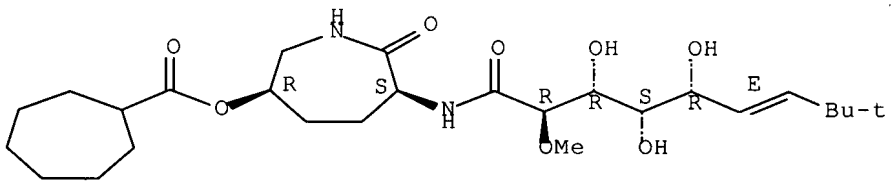
RN 270902-52-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclopentylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-53-9 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cycloheptylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

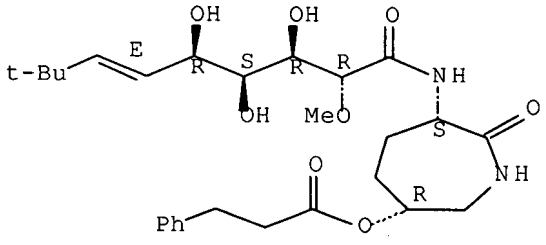
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-54-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-(1-oxo-3-phenylpropoxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

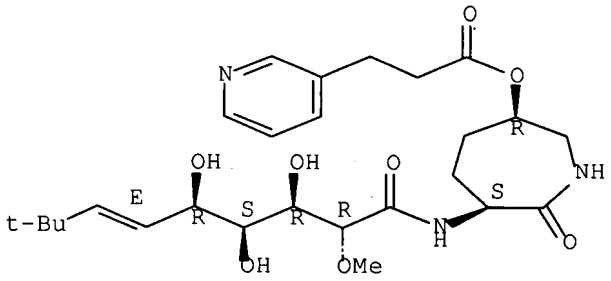
Absolute stereochemistry.

Double bond geometry as shown.



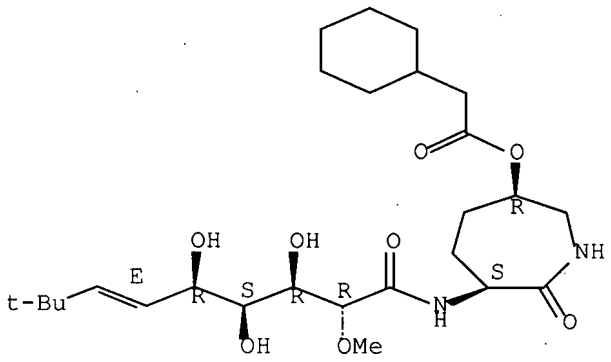
RN 270902-55-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[1-oxo-3-(3-pyridinyl)propoxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



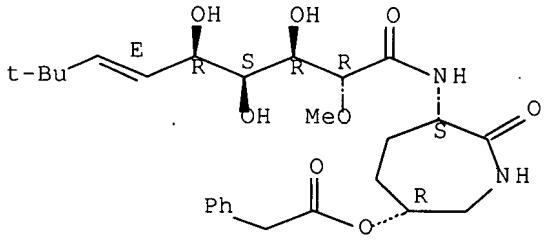
RN 270902-56-2 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylacetyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



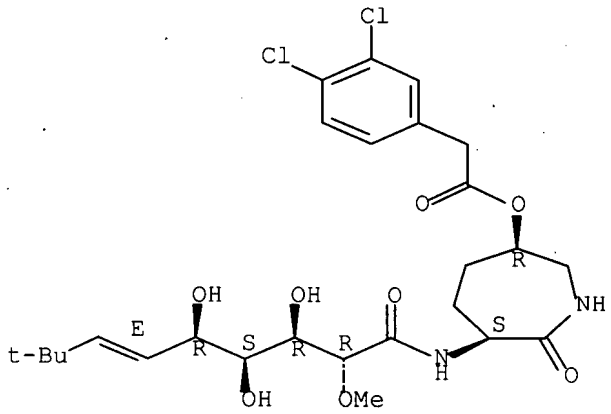
RN 270902-57-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(phenylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



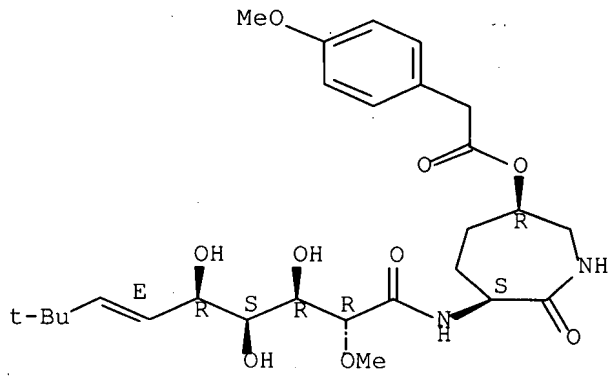
RN 270902-58-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(3,4-dichlorophenyl)acetyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



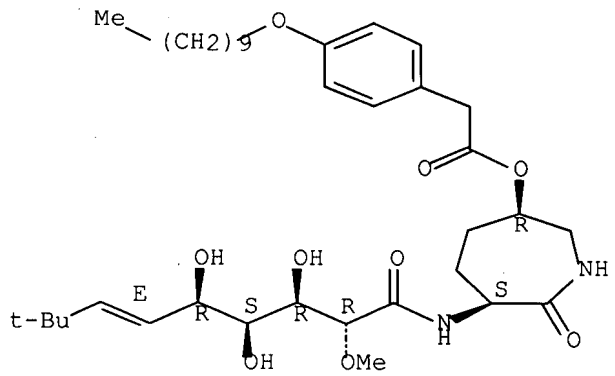
RN 270902-59-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[[(4-methoxyphenyl)acetyl]oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



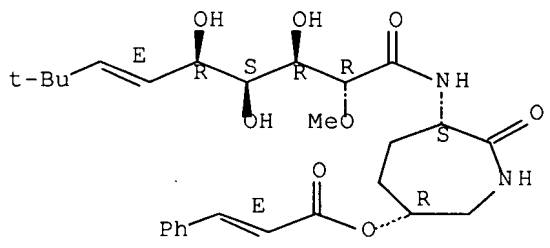
RN 270902-60-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[[4-(decyloxy)phenyl]acetyl]oxy]hexa hydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



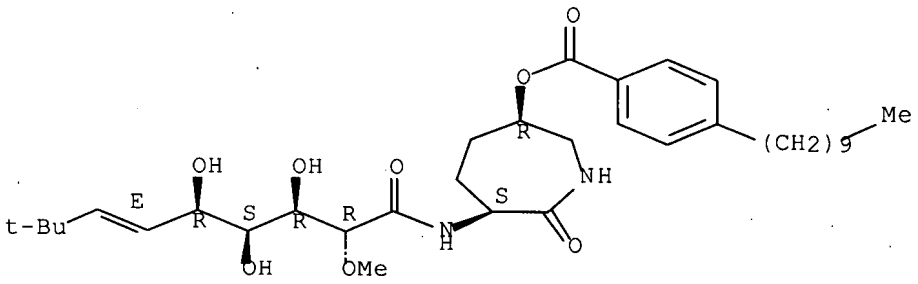
RN 270902-61-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



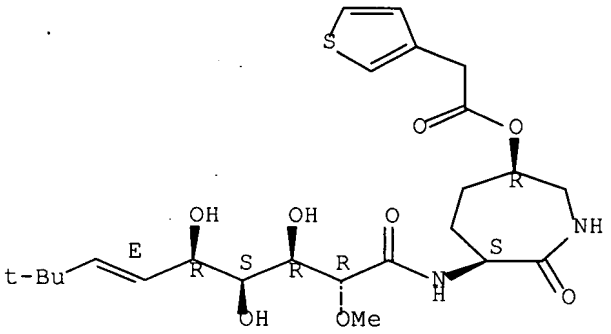
RN 270902-62-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(4-decylbenzoyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



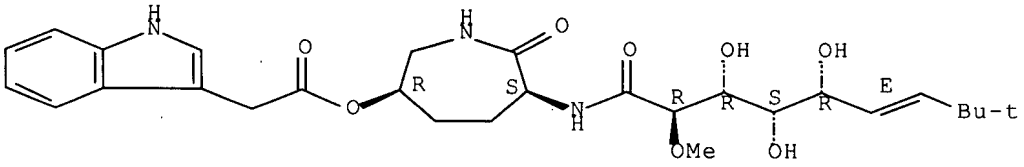
RN 270902-63-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(3-thienylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-64-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[(1H-indol-3-ylacetyl)oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

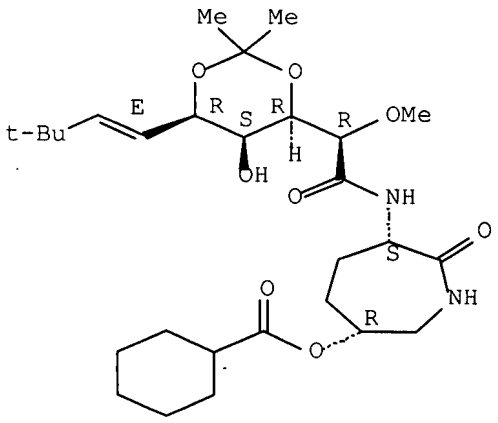


IT 270902-71-1P 270902-74-4P 270902-75-5P
270902-76-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and use of substituted caprolactams as antitumor agents)

RN 270902-71-1 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

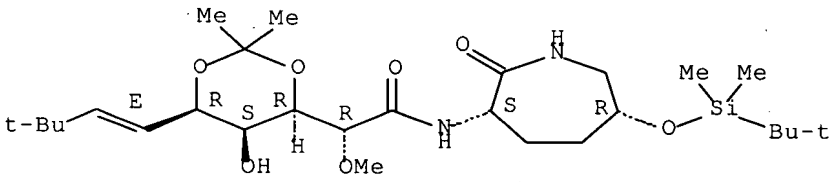
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 270902-74-4 CAPLUS

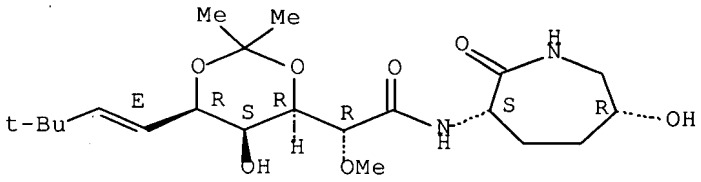
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



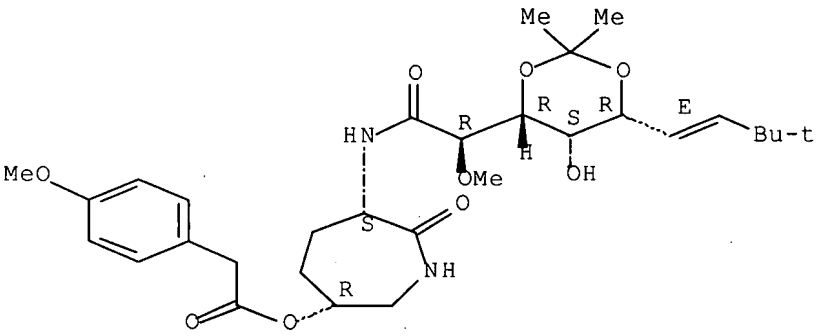
RN 270902-75-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



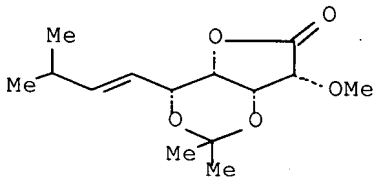
RN 270902-76-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[[(4-methoxyphenyl)acetyl]oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

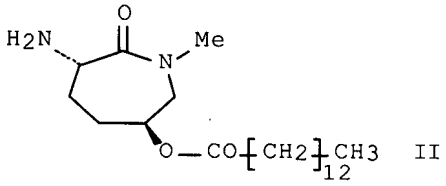


RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 28 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:136212 CAPLUS Full-text
DN 134:296016
TI Total Syntheses of Bengamides B and E
AU Kinder, Frederick R., Jr.; Wattanasin, Sompong; Versace, Richard W.; Bair, Kenneth W.; Bontempo, John; Green, Michael A.; Lu, Yansong J.; Marepalli, H. Rao; Phillips, Penny E.; Roche, Didier; Tran, Long D.; Wang, RunMing; Waykole, Liladhar; Xu, David D.; Zabludoff, Sonya
CS Oncology Department, Novartis Pharmaceuticals Corporation, Summit, NJ, 07901, USA
SO Journal of Organic Chemistry (2001), 66(6), 2118-2122
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:296016
GI



I

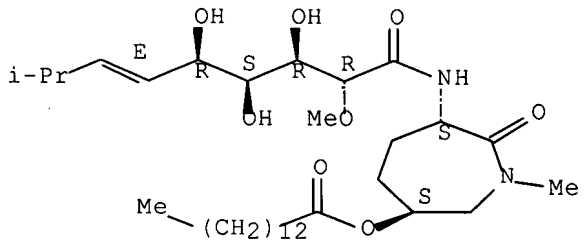


II

AB Total syntheses of the cytotoxic marine natural products bengamides B and E are described. Both bengamides are prepared via amide coupling of a protected polyhydroxylated lactone intermediate I with a suitably substituted aminocaprolactam intermediate. Lactone I is prepared in five steps from com. available α-D-glucoheptonic γ-lactone. The key reactions are a selective deprotection of a 1,2-acetonide in the presence of a 1,3-acetonide and an (E)-selective olefination of an unstable aldehyde using a gem-dichromium reagent. The bengamide B lactam intermediate II is prepared in seven steps from com. available (5R)-5-hydroxy-L-lysine. The desired S-configuration at the γ-OH lactam position is established using the Mitsunobu reaction.

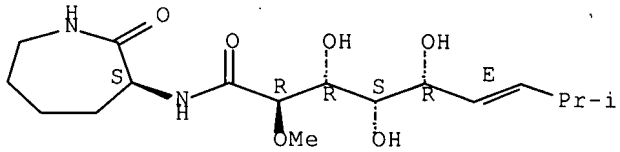
IT 104947-69-5P, (+)-Bengamide B 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(total syntheses of bengamides B and E)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

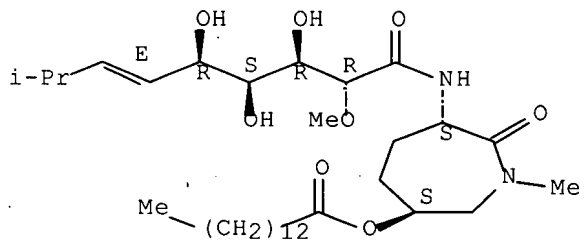
Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

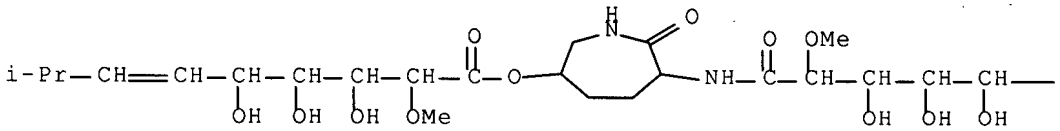
L10 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:72694 CAPLUS Full-text
DN 134:260872
TI Bengamides revisited: new structures and antitumor studies
AU Thale, Zia; Kinder, Frederick R.; Bair, Kenneth W.; Bontempo, John; Czuchta, Ania M.; Versace, Richard W.; Phillips, Penny E.; Sanders, Miranda L.; Wattanasin, Sompong; Crews, Phillip
CS Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA, 95064, USA
SO Journal of Organic Chemistry (2001), 66(5), 1733-1741
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:260872
AB The structural chemical and biol. activity of the bengamide class of compds. have been further characterized. Exts. prepared from recollected Jaspis cf. coricea from five sites in Fiji were pooled. Six new bengamides, M (7b), N (8a), O (8b), P (9a), Q (9b), and R (10), were identified, accompanied by the known bengamides A (1a), B (1b), E (3a), F (3b), Y (5), Z (6), L (7a), G (11a), H (11b), and I (12). The structures of the new compds. were determined from spectroscopic data, and some were addnl. confirmed by semisynthesis. Cytotoxicity screening data were obtained from the NCI-DTP 60 cell screen for bengamides A, B, and P. Bengamides A and B were more potent than bengamide P, with average IC50 values of 0.046, 0.011, and 2.70 FM, resp. The in vitro antitumor activity against MDA-MB-435 human mammary carcinoma was also determined for natural bengamides A, B, E, F, P, M, O, and Z and for synthetic samples of B and O. The best activity was observed for the natural bengamides A (IC50 = 1 nM) and O (IC50 = 0.3 nM).
IT 104947-69-5P, Bengamide B 104975-72-6P, Bengamide C
118477-02-4P, Bengamide D 118477-03-5P, Bengamide E
118477-04-6P, Bengamide F 118477-09-1P, Bengamide Y
118477-10-4P, Bengamide Z 193894-94-9P, Bengamide G
193894-95-0P, Bengamide H 193894-96-1P, Bengamide I
226922-85-6P, Bengamide L 331765-19-6P, Bengamide M
331766-12-2P, Bengamide O 331766-63-3P, Bengamide Q
331766-64-4P, Bengamide R 331766-65-5P, Bengamide N
331766-67-7P, Bengamide P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antitumor SAR of sponge-derived natural bengamides)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 104975-72-6 CAPLUS
CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



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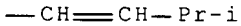
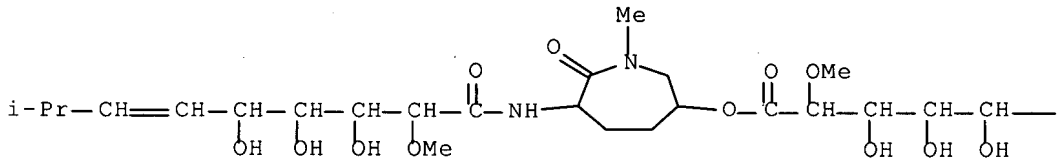


RN 118477-02-4 CAPLUS
CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-1-methyl-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



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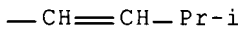
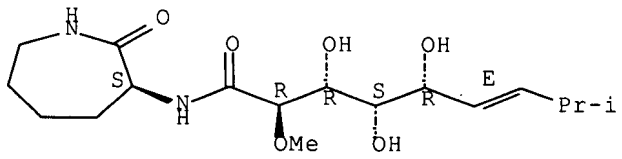
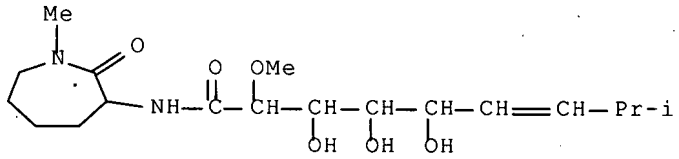


RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

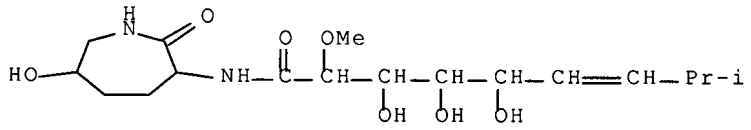
Absolute stereochemistry.
Double bond geometry as shown.



RN 118477-04-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

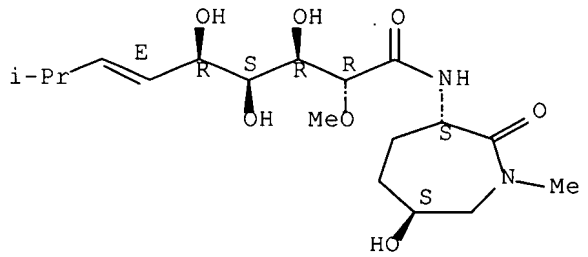


RN 118477-09-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

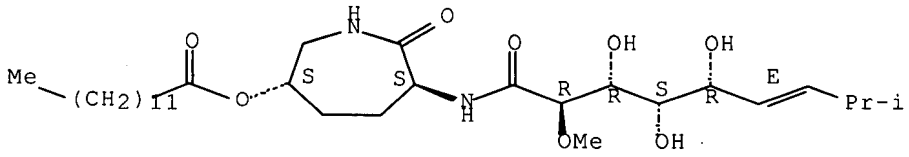
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 193894-94-9 CAPLUS

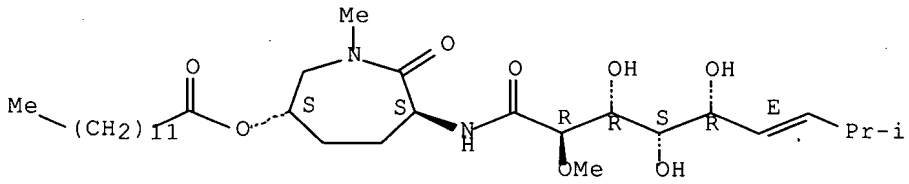
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotridecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



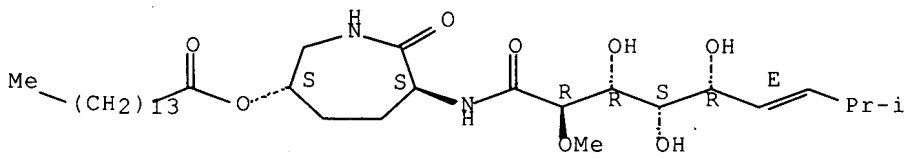
RN 193894-95-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotridecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



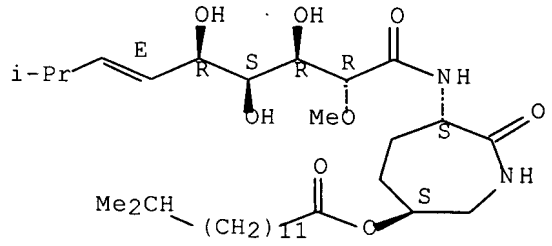
RN 193894-96-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxopentadecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



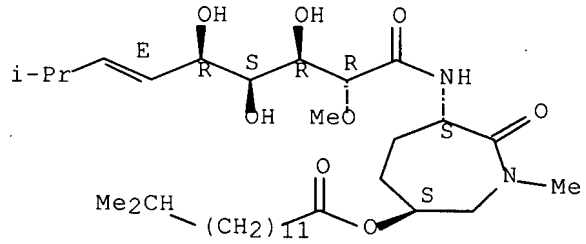
RN 226922-85-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-[(13-methyl-1-oxotetradecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



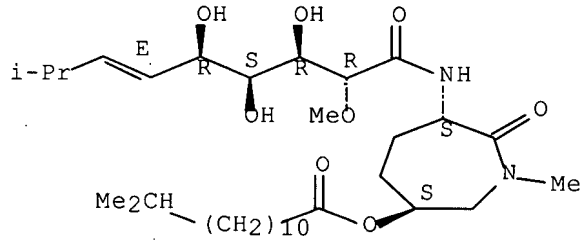
RN 331765-19-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-6-[(13-methyl-1-oxotetradecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 331766-12-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-6-[(12-methyl-1-oxotridecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

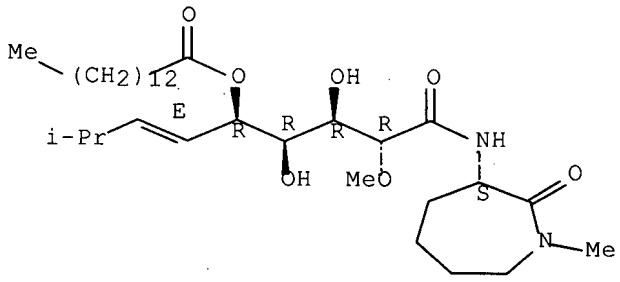
Absolute stereochemistry.
Double bond geometry as shown.



RN 331766-63-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-tetradecanoate, (6E)- (9CI) (CA INDEX NAME)

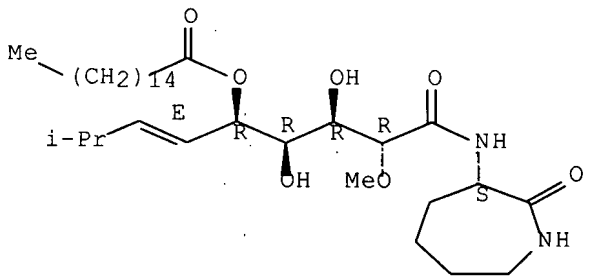
Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



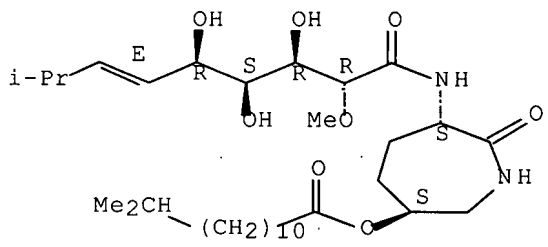
RN 331766-64-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 5-hexadecanoate, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 331766-65-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-[(12-methyl-1-oxotridecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

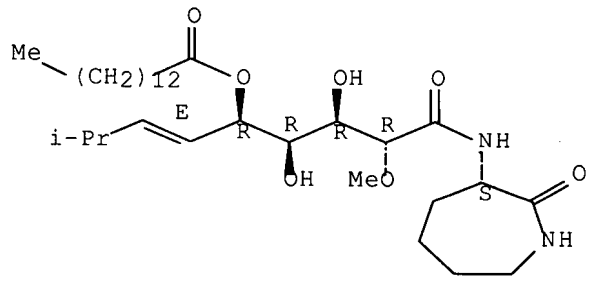
Absolute stereochemistry.
Double bond geometry as shown.



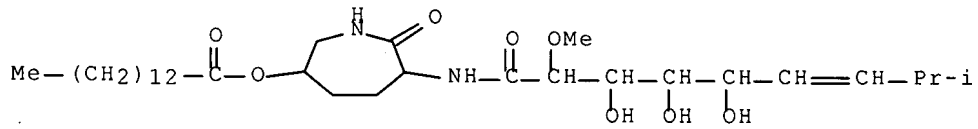
RN 331766-67-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-

azepin-3-yl]-8-methyl-2-O-methyl-, 5-tetradecanoate, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

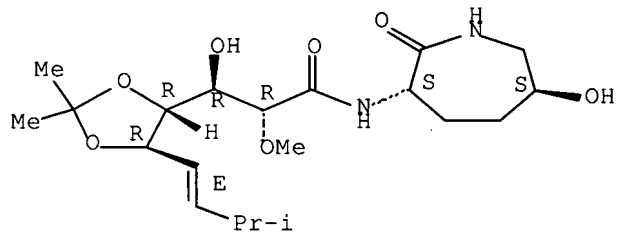


IT 104947-68-4, Bengamide A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor SAR of sponge-derived natural bengamides)
RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



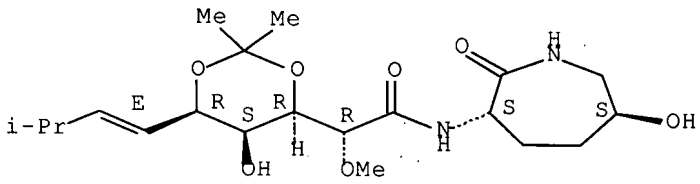
IT 331754-55-3P 331754-56-4P 331754-57-5P
331754-58-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(antitumor SAR of sponge-derived natural bengamides)
RN 331754-55-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



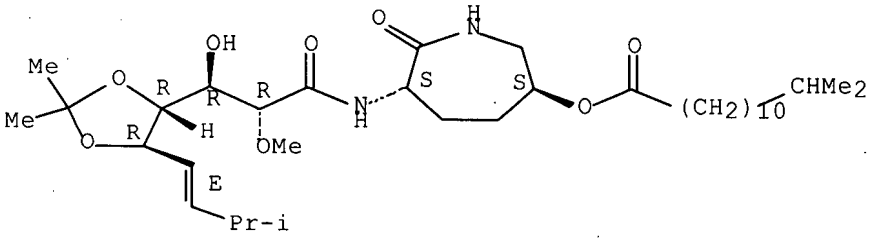
RN 331754-56-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



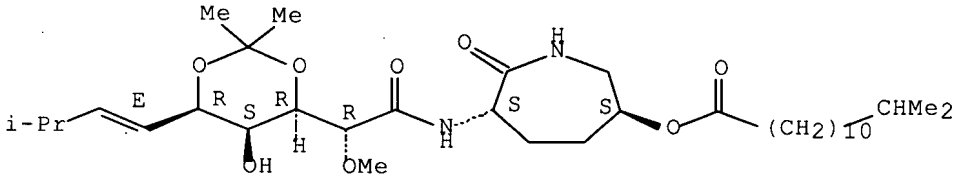
RN 331754-57-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-[(12-methyl-1-oxotridecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 331754-58-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-[(12-methyl-1-oxotridecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:351502 CAPLUS Full-text
DN 133:4993
TI Preparation of substituted caprolactams as anticancer agents
IN Kinder, Frederick Ray, Jr.; Bair, Kenneth Walter; Jagoe, Christopher Turchik; Versace, Richard William; Wattanasin, Sompong
PA Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.
SO PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000029382	A1	20000525	WO 1999-EP8767	19991115
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	BR 9915436	A	20010807	BR 1999-15436	19991115
	EP 1131297	A1	20010912	EP 1999-957309	19991115
	EP 1131297	B1	20040414		
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	ES 2221463	T3	20041216	ES 1999-957309	19991115
	ZA 2001003419	A	20020626	ZA 2001-3419	20010426
	NO 2001002428	A	20010717	NO 2001-2428	20010516
PRAI	US 1998-193354	A	19981117		
	WO 1999-EP8767	W	19991115		

OS MARPAT 133:4993
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The caprolactams I (R1 = (C1-6)alkyl or (C3-6)cycloalkyl; R2 = H, (C1-6)alkyl; X = (C1-12)alkylene, (C2-12)alkenylene; or (C2-12)alkynylene; m is 0 or 1; and R3 is (C3-8)cycloalkyl; or an aromatic ring system selected from Q, Q1, Q2, Q3 where R4 = H, Cl, or methoxy; R5 = H, Cl, (C1-18)alkyl or (C1-18)alkoxy, and Z = O, S, NH, or NMe) and their pharmaceutically acceptable acid addition salts were prepared for pharmaceutical compns. in treating tumors. Thus, (6E)-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl- 3,5-O-(1-methylethylidene)-gulo-non-6-enonic acid lactone II, prepared in 5 steps from α-D-glucopheptonic γ-lactone was treated with (3S,6R)-3-aminohexahydro-6-(cyclohexanecarbonyloxy)-

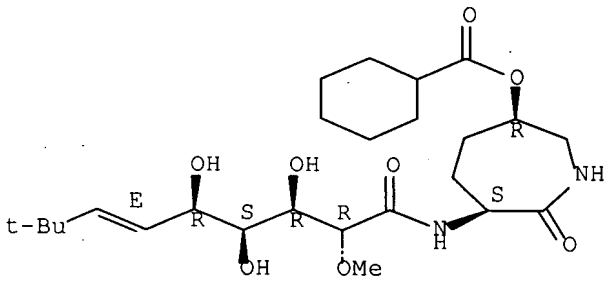
2H-azepin-2-one to give the azepinylnonenamide III. The IC50 of III against MDA-MB-435 cells was 0.068 μM .

IT 270902-51-7P 270902-52-8P 270902-53-9P
270902-54-0P 270902-55-1P 270902-56-2P
270902-57-3P 270902-58-4P 270902-59-5P
270902-60-8P 270902-61-9P 270902-62-0P
270902-63-1P 270902-64-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted caprolactams as antitumor agents)

RN 270902-51-7 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

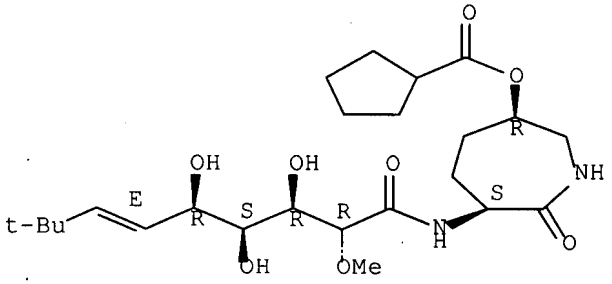
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-52-8 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclopentylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

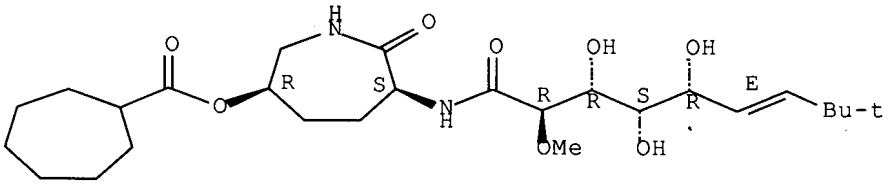


RN 270902-53-9 CAPLUS

CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cycloheptylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

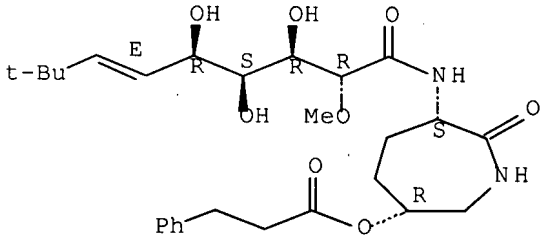
Absolute stereochemistry.

Double bond geometry as shown.



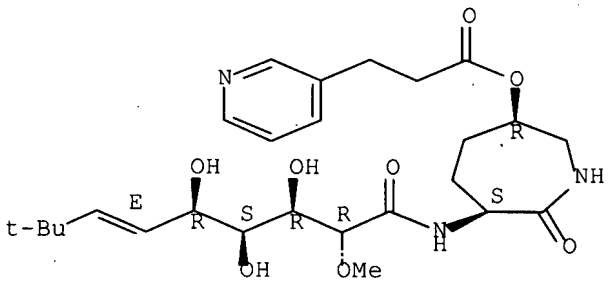
RN 270902-54-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-(1-oxo-3-phenylpropoxy)-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



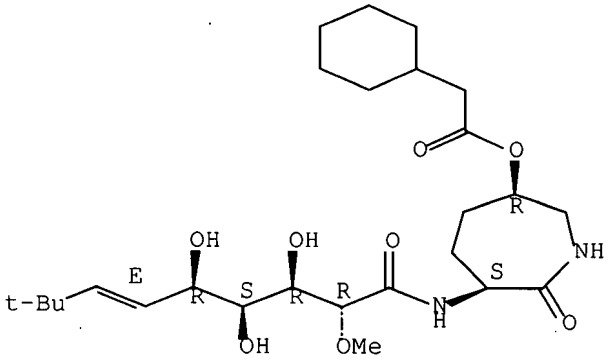
RN 270902-55-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[1-oxo-3-(3-pyridinyl)propoxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



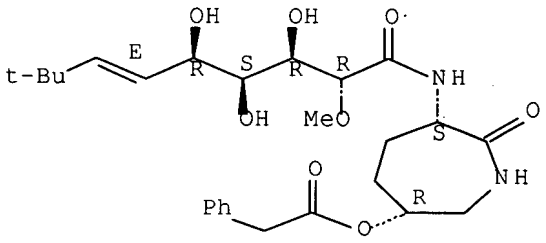
RN 270902-56-2 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylacetyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



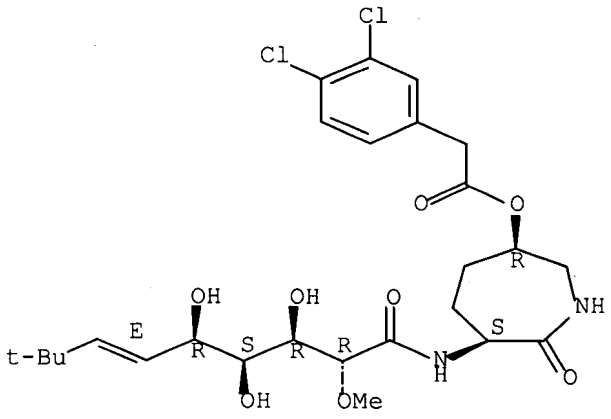
RN 270902-57-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(phenylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



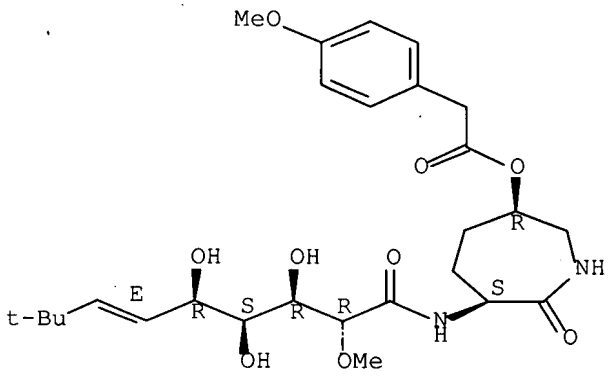
RN 270902-58-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(3,4-dichlorophenyl)acetyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



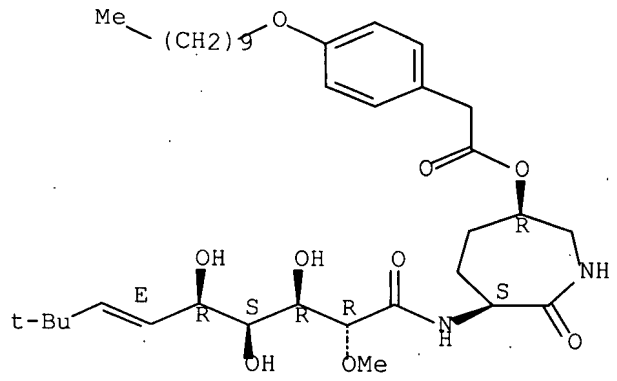
RN 270902-59-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[[(4-methoxyphenyl)acetyl]oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



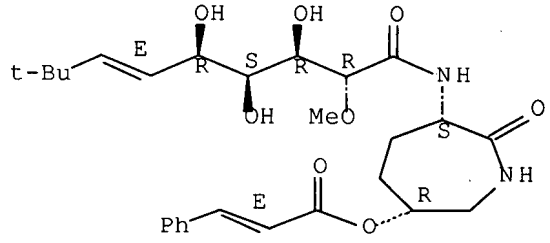
RN 270902-60-8 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[[[4-(decyloxy)phenyl]acetyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



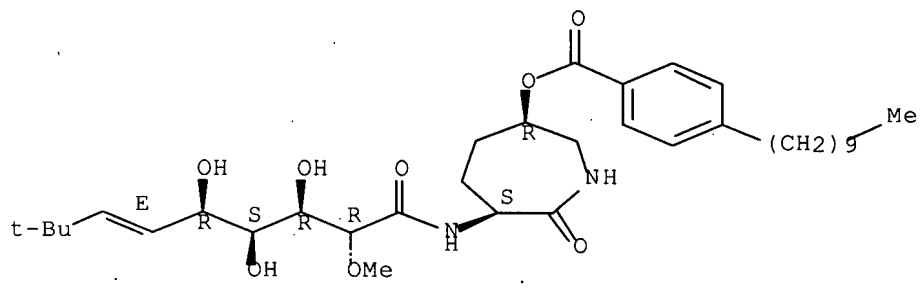
RN 270902-61-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[[(2E)-1-oxo-3-phenyl-2-propenyl]oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-62-0 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(4-decylbenzoyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

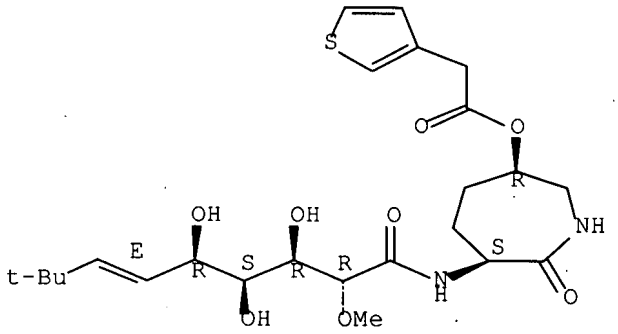
Absolute stereochemistry.
Double bond geometry as shown.



RN 270902-63-1 CAPLUS

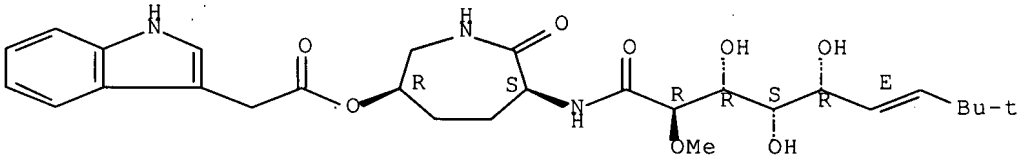
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-2-oxo-6-[(3-thienylacetyl)oxy]-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



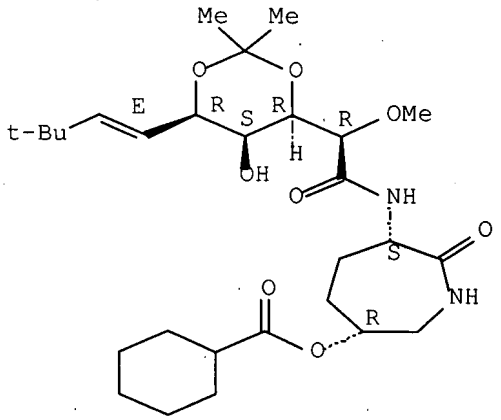
RN 270902-64-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[(1H-indol-3-ylacetyl)oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



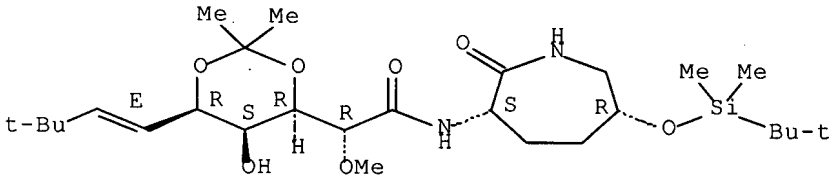
IT 270902-71-1P 270902-74-4P 270902-75-5P
270902-76-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted caprolactams as antitumor agents)
RN 270902-71-1 CAPLUS
CN D-gulo-Non-6-enonamide, N-[(3S,6R)-6-[(cyclohexylcarbonyl)oxy]hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



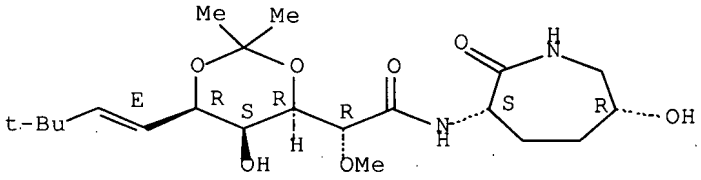
RN 270902-74-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-6-[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexahydro-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



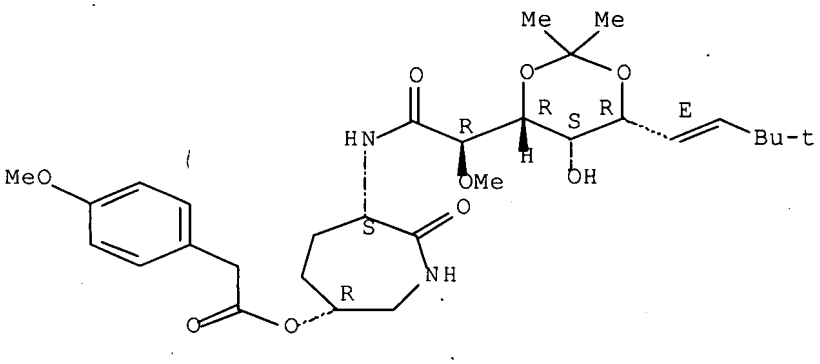
RN 270902-75-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



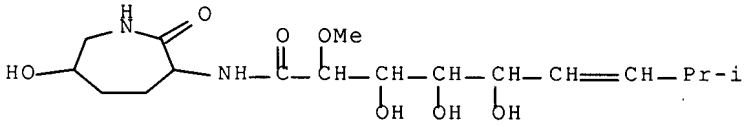
RN 270902-76-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6R)-hexahydro-6-[[(4-methoxyphenyl)acetyl]oxy]-2-oxo-1H-azepin-3-yl]-8,8-dimethyl-2-O-methyl-3,5-O-(1-methylethylidene)-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



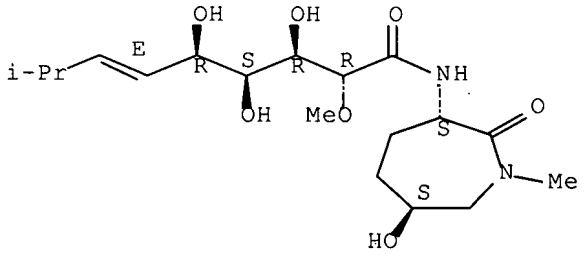
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 31 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:680984 CAPLUS Full-text
DN 132:30415
TI Cytotoxic Metabolites from an Australian Collection of the Sponge Jaspis Species
AU Groweiss, Amiram; Newcomer, Joshua J.; O'Keefe, Barry R.; Blackman, Adrian; Boyd, Michael R.
CS Laboratory of Drug Discovery Research and Development Developmental Therapeutics Program Division of Cancer Treatment and Diagnosis National Cancer Institute, Frederick Cancer Research and Development Center, Frederick, MD, 21702-1201, USA
SO Journal of Natural Products (1999), 62(12), 1691-1693
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
AB Three new natural products, bengamide Y (1), bengamide Z (3), and bengazole Z (5), were isolated from the aqueous extract of an Australian collection of the sponge Jaspis sp. Their structures were solved by spectroanal. methods and by comparison of their spectral data with known bengamides and bengazoles that were reported from the same genus. Bengamides Y (1) and Z (3) showed a striking differential cytotoxicity pattern against a panel of 10 human tumor cell lines, with closely related cell lines (e.g., SNB-19 and SNB-75) displaying significant differences in sensitivity.
IT 118477-09-1, Bengamide Y 118477-10-4, Bengamide Z
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cytotoxic metabolites from Australian collection of sponge Jaspis sp.)
RN 118477-09-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



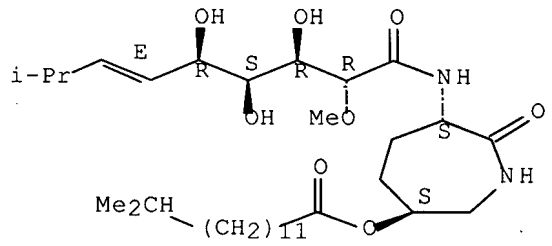
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:222774 CAPLUS Full-text
DN 131:29932
TI Antifungal Metabolites from the Marine Sponge Pachastrissa sp.: New Bengamide and Bengazole Derivatives
AU Fernandez, Rogelio; Dherbomez, Michel; Letourneux, Yves; Nabil, Mohamed; Verbist, Jean Francois; Biard, Jean Francois
CS Laboratoire SESNAB Pole Science, Universite de La Rochelle, La Rochelle, 17042, Fr.
SO Journal of Natural Products (1999), 62(5), 678-680
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

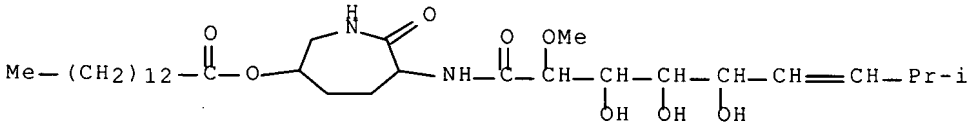
AB This paper reports the studies of components of an undescribed sponge in the genus Pachastrissa sp., collected along the Djibouti coast. The extract showed activity against Candida albicans. Six new bengazoles [I; R1 = CO(CH2)14Me, R2 = H; R1 = H, R2 = CO(CH2)14Me; R1 = CO(CH2)12CHMe2, R2 = H; R1 = H, R2 = CO(CH2)12CHMe2; R1 = CO(CH2)13Me, R2 = H; R1 = H, R2 = CO(CH2)13Me] and a new bengamide, named bengamide L [II; R3 = CO(CH2)11CHMe2, R4 = H], in addition to the known bengazoles [I; R1 = CO(CH2)11CHMe2, R2 = H; R1 = H, R2 = CO(CH2)11CHMe2; R1 = CO(CH2)12Me, R2 = H; R1 = H, R2 = CO(CH2)12Me; R1 = R2 = H], bengamides A [II; R3 = CO(CH2)12Me, R4 = H], B [II; R3 = CO(CH2)12Me, R4 = Me], E [II; R3 = R4 = H], and F [II; R3 = H, R4 = Me], and lactone III are described in this paper. All structures were determined on the basis of spectroscopic studies.
IT 226922-85-6P, Bengamide L
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and structure of new bengamide and antifungal bengazole derivs. from the marine sponge Pachastrissa sp)
RN 226922-85-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-[(13-methyl-1-oxotetradecyl)oxy]-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



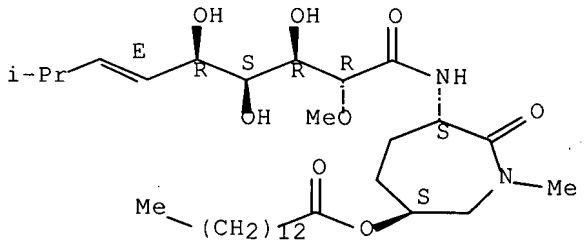
IT 104947-68-4P, Bengamide A 104947-69-5P, Bengamide B
118477-03-5P, Bengamide E 118477-04-6P, Bengamide F
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and structure of new bengamide and antifungal bengazole derivs. from the marine sponge Pachastrissa sp)

RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



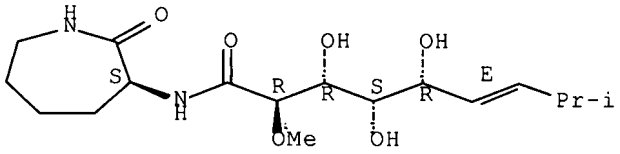
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

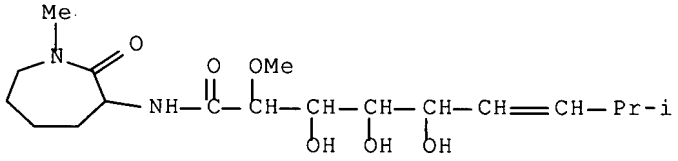


RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

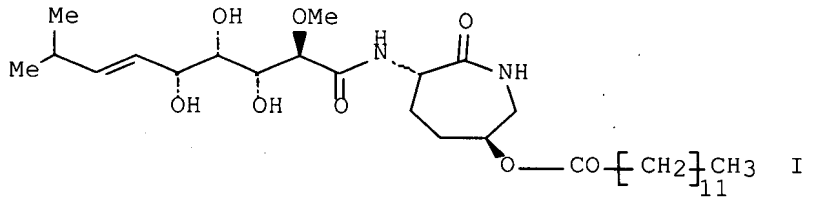


RN 118477-04-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

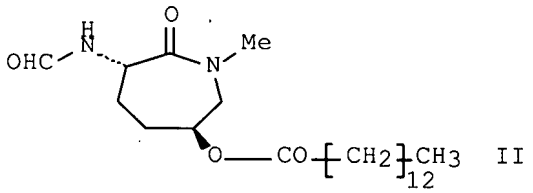


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1997:496874 CAPLUS Full-text
DN 127:173995
TI Bengamides and related new amino acid derivatives from the New Caledonian marine sponge Jaspis carteri
AU D'Auria, M. Valeria; Giannini, Clelia; Minale, Luigi; Zampella, Angela; Debitus, Cecile; Frostin, Maryvonne
CS Dipartimento di Chimica delle Sostanze Naturali, Universita degli Studi di Napoli Federico II, Naples, 80131, Italy
SO Journal of Natural Products (1997), 60(8), 814-816
CODEN: JNPRDF; ISSN: 0163-3864
PB American Chemical Society
DT Journal
LA English
GI



I

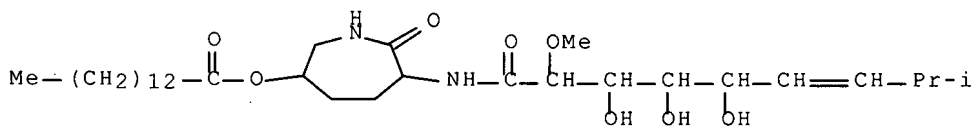


II

AB Five new amino acid derivs. were isolated from the New Caledonian sponge Jaspis carteri, together with known bengamides A and B. The structures of the new compds. were determined by interpretation of their spectral data and by comparison with spectral data of known bengamides. Bengamides G (I), and H, I, and J are simply the tridecanoate and pentadecanoate analogs of the original bengamides A and B, whereas bengamide K (II) is a caprolactam formamide derivative of bengamide B.

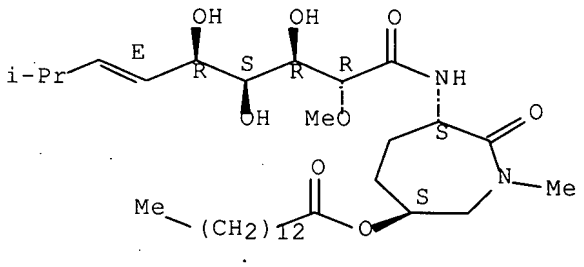
IT 104947-68-4P, Bengamide A 104947-69-5P, Bengamide B
193894-94-9P, Bengamide G 193894-95-0P, Bengamide H
193894-96-1P, Bengamide I 193894-97-2P, Bengamide J
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(bengamide isolation and structural characterization and anticandidal activity from marine sponge Jaspis carteri)

RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



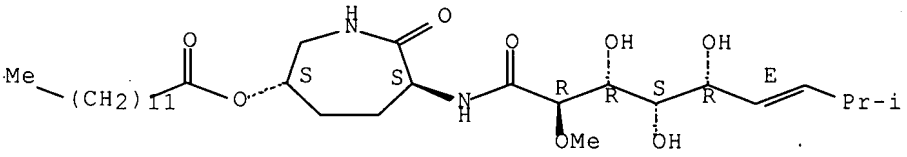
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



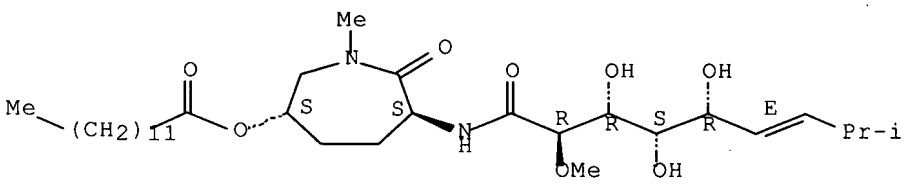
RN 193894-94-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotridecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



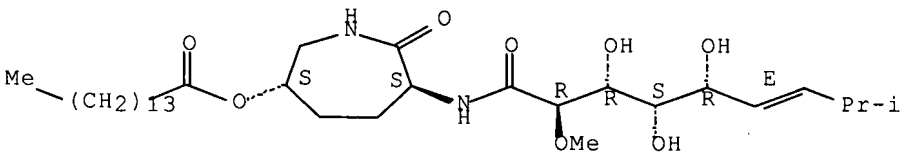
RN 193894-95-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotridecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



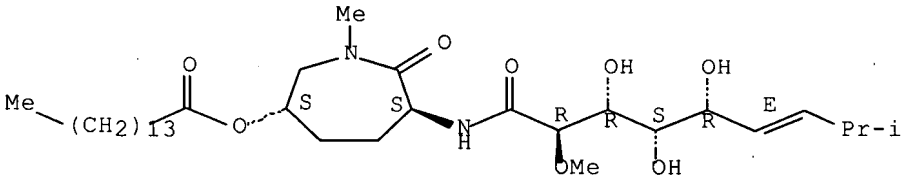
RN 193894-96-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxopentadecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 193894-97-2 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxopentadecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

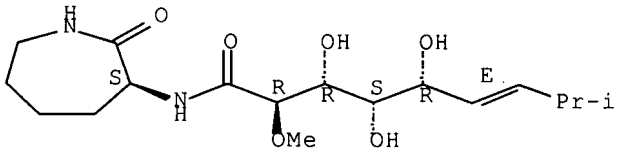
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1997:250459 CAPLUS Full-text
DN 126:293199
TI Studies on highly stereoselective syntheses of bioactive compounds based on alkyne-Co and benzaldehyde-Cr complexes
AU Mukai, Chisato
CS Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan
SO Yakugaku Kenkyu no Shinpo (1997), Volume Date 1996, 13, 93-103
CODEN: YAKSEY; ISSN: 0914-4544
PB Yakugaku Kenkyu Shorei Zaidan
DT Journal; General Review
LA Japanese
AB A review with 17 refs. Alkyne-Co2(CO)6 complex and benzaldehyde-Cr(CO)3 complex have been shown to be useful substrates for highly selective reactions. Some inherent properties of these complexes have been utilized for development of highly syn-selective aldol reaction as well as antiselective aldol reaction. On the basis of these newly developed aldol reactions, several bioactive species like PS-5, bengamide E, antitumor styryllactones have been synthesized in a highly stereocontrolled manner.
IT 118477-03-5P, Bengamide e
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(highly stereoselective syntheses of bioactive compds. based on alkyne-Co and benzaldehyde-Cr complexes)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

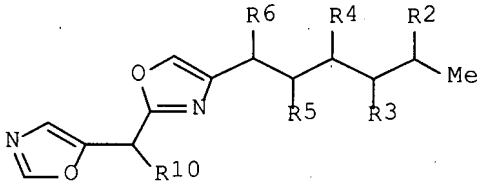
Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:171805 CAPLUS Full-text
DN 124:232136
TI Oxazole derivatives as antitumoral agents
IN Gravalos, Dolores G.; Kashman, Yoel; Rudi, Amira; De La Fuente, Jesus Angel
PA Pharma Mar, S.A., Spain
SO Eur. Pat. Appl., 10 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 687673	A1	19951220	EP 1995-304021	19950609
R: BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
CA 2151635	A1	19951215	CA 1995-2151635	19950613
JP 08176124	A	19960709	JP 1995-147624	19950614
PRAI GB 1994-11841	A	19940614		

OS MARPAT 124:232136
GI



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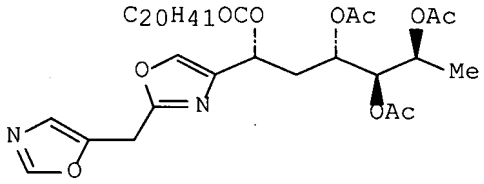


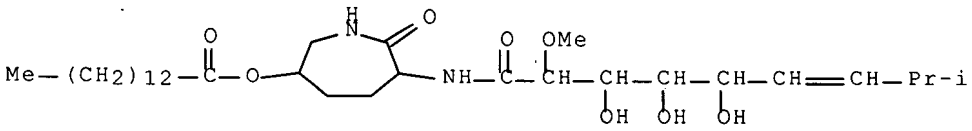
II

AB New antitumoral compds. are of formula I: where R2, R3, R4, R5, R67, and R10 are the same of different and each represents a hydrogen atom, an alkyl group of 1-6 carbon atoms, a hydroxy group or an acyloxy group R-(C = O)-O- (where R-(C = O)- is an acyl group or 1-26 carbon atoms); provided that at least one of R2, R3, R4, R5, R6 and R10 is an acyloxy group R-(C = O)-O- (where R-(C = O)- is an acyl group of 1-26 carbon atoms) and further provided that at least one of R3, R3, R4, R5, R6, and R10 is an acyloxy group R-(C = O)-O- (where R-(C = O)- is an acyl group of 10-25 carbon atoms); with the exception of the tetraacetate of bengazole A and the tetraacetate of bengazole B. The lead to these compds. is provided by digonazole triacetate of formula (II), obtained from digonazole which may itself be extracted from Jaspis digonoxea.

IT 104947-68-4, Bengamide A 104947-69-5, Bengamide B
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(preparation of oxazole derivs. as antitumoral agents)

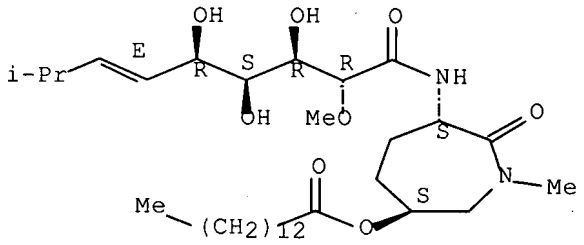
RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI)

(CA INDEX NAME)



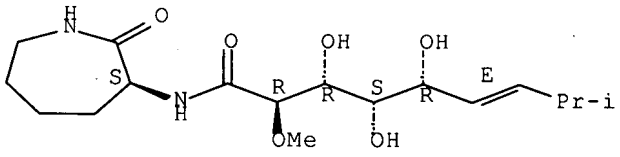
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

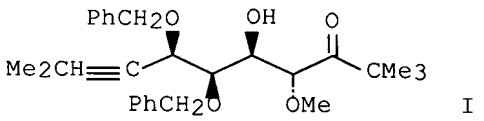


L10 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1996:93820 CAPLUS Full-text
DN 124:202739
TI Development of highly stereoselective and regioselective reactions based on the alkyne-Co2(CO)6 complexes
AU Mukai, Chisato; Hanaoka, Miyoji
CS Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan
SO Synlett (1996), (1), 11-17
CODEN: SYNLES; ISSN: 0936-5214
PB Thieme
DT Journal; General Review
LA English
AB A review with 28 refs., highly syn-selective aldol reaction of the propynal-Co2(CO)6 complexes with silyl enol nucleophiles under the Mukaiyama conditions was developed. Based on the newly developed stereoselective reactions, stereoselective syntheses of (±)-PS-5, (±)-blastmycinone, and (+)-bengamide E was achieved. The novel endo mode ring closure of the epoxy-alcs. via the corresponding cobalt complexes was described. In this cyclization., complete regioselectivity was attained and the reaction proceeded with retention of configuration at the propynyl position of tetrahydropyran and THF derivs.
IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(development of highly stereoselective and regioselective reactions based on alkyne-cobalt carbonyl complexes)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:953999 CAPLUS Full-text
DN 124:55662
TI Highly stereocontrolled total synthesis of (+)-bengamide E
AU Mukai, Chisato; Moharram, Sameh M.; Kataoka, OSamu; Hanaoka, Miyoji
CS Fac. Pharmaceutical Sci., Kanazawa Univ., Kanazawa, 920, Japan
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1995), (22), 2849-54
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 124:55662
GI



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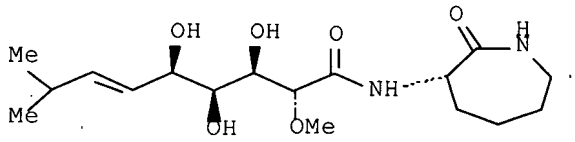
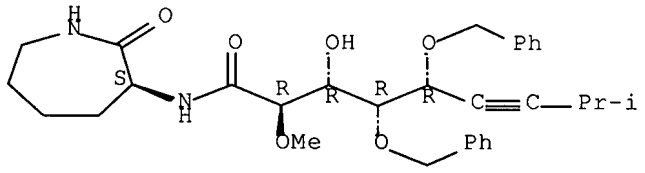


II

AB Diisopropyl D-tartrate was efficiently transformed into the hexacarbonyl dicobalt complexed aldehyde. A highly stereocontrolled aldol reaction of the complexed aldehyde with the MeOCH:C(SCMe3)OSiMe3 in the presence of tin(IV) chloride provided, after decomplexation, the aldol adduct I as the sole product, which was subsequently converted into (+)-bengamide E (II).

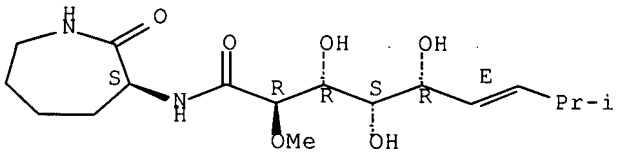
IT 171863-69-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(highly stereocontrolled total synthesis of (+)-bengamide E)
RN 171863-69-7 CAPLUS
CN D-gulo-Non-6-ynonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4,5-bis-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 118477-03-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(highly stereocontrolled total synthesis of (+)-bengamide E)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.


H
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OH
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OH
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OH
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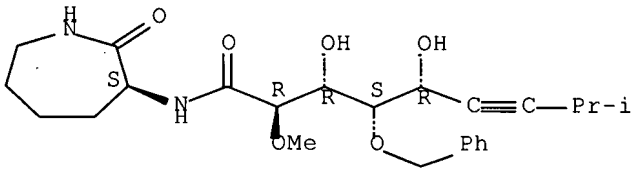
E
Pr-i

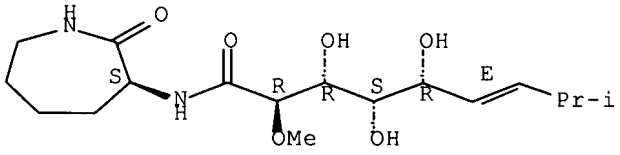
L10 ANSWER 38 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:827462 CAPLUS Full-text
DN 124:29246
TI An efficient method for the optical resolution of 3-hydroxy-2-substituted-4-alkynoates: a highly stereoselective total synthesis of (+)-bengamide E1
AU Mukai, Chisato; Kataoka, Osamu; Hanaoka, Miyoji
CS Fac. Pharmaceutical Sci., Kanazawa Univ., Kanazawa, 920, Japan
SO Journal of Organic Chemistry (1995), 60(18), 5910-18
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 124:29246
AB A novel procedure for the optical resolution of 3-hydroxy-2-substituted-4-alkynoates and its application to the stereoselective total synthesis of (+)-bengamide E are described. 3-Hydroxy-2-substituted-4-alkynoates, derived from the aldol reaction of cobalt-complexed propynals with ketene O-silyl O,S-acetals, were easily resolved by the formation of a chiral carbamate followed by cobalt complexation. Chiral-2-(benzyloxy)-3-hydroxy- 4-alkynoate derivs. thus obtained were used as starting materials for a highly stereoselective total synthesis of (+)-bengamide E.
IT 160840-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(resolution of substituted hydroxyalkynoates via chiral carbamates in asym. total synthesis of bengamide E)
RN 160840-67-5 CAPLUS
CN D-gulo-Non-6-ynonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

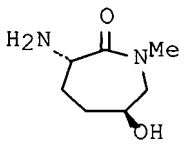


IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(resolution of substituted hydroxyalkynoates via chiral carbamates in asym. total synthesis of bengamide E)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:271239 CAPLUS Full-text
DN 122:314985
TI Stereoselective conversion of L-quebrachitol into a novel hydroxylated caprolactam: total synthesis of beingamide B
AU Chida, Noritaka; Tobe, Takahiko; Murai, Katsuyuki; Yamazaki, Kaori; Ogawa, Seiichiro
CS Faculty of Science and Technology, Keio University, Yokohama, 223, Japan
SO Heterocycles (1994), 38(11), 2383-8
CODEN: HTCYAM; ISSN: 0385-5414
PB Japan Institute of Heterocyclic Chemistry
DT Journal
LA English
OS CASREACT 122;314985
GI



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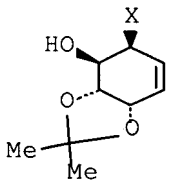
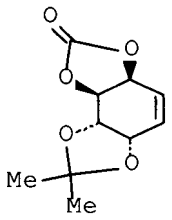


II



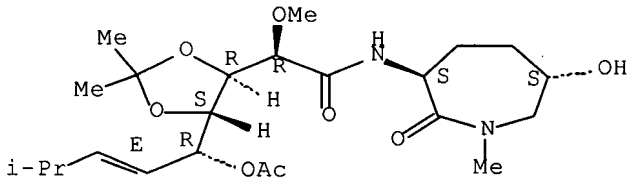
III

AB The stereoselective synthesis of the novel marine natural product, bengamide B, starting from L-quebrachitol, is described. The hydroxylated caprolactam portion (I) in quebrachitol was prepared from (+)-conduramine derivative (II) whose amino functionality was introduced stereoselectively by palladium-catalyzed azidation of a chiral cyclohexene (III) derived from L-quebrachitol.

IT 163072-72-8P 163072-73-9P 163072-74-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation as intermediate for beingamide B)

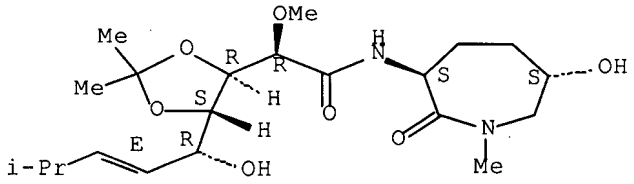
RN 163072-72-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, 5-acetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



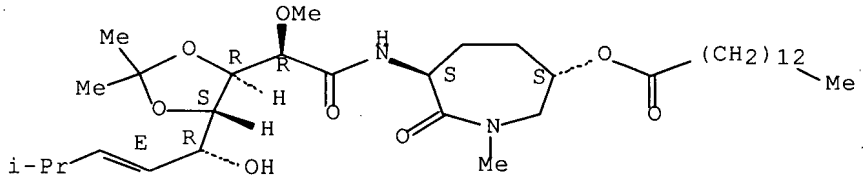
RN 163072-73-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



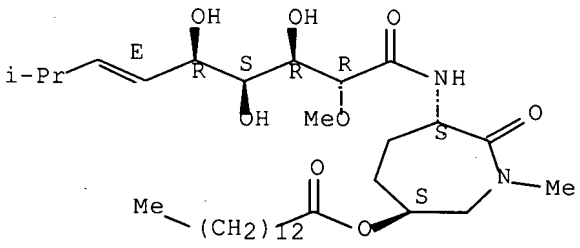
RN 163072-74-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

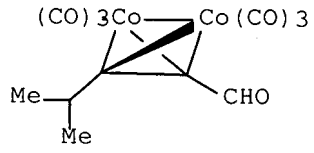


IT 104947-69-5P, Bengamide b
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective conversion of L-quebrachitol into a novel hydroxylated caprolactam: total synthesis of beingamide B)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

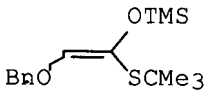
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.


OH
OH
O
E
i-Pr
R
S
R
R
NH
OH
MeO
S
O
N
Me
O
S
Me
(CH2)12
O

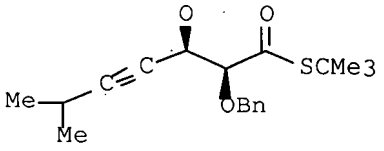
L10 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:86526 CAPLUS Full-text
DN 122:133722
TI A cobalt-complexed propynal in organic synthesis: a highly stereoselective total synthesis of begamide E
AU Mukai, Chisato; Kataoka, Osamu; Hanaoka, Miyoji
CS Fac. Pharm Sci., Kanazawa Univ., Kanazawa, 920, Japan
SO Tetrahedron Letters (1994), 35(37), 6899-902
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 122:133722
GI



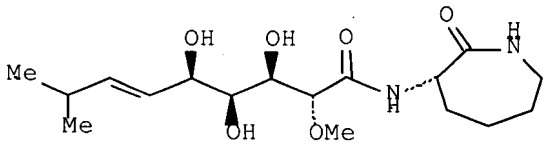
I



II



III



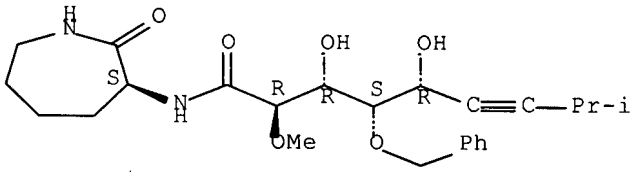
IV

AB A highly stereoselective aldol reaction of the cobalt-complexed 4-methylpent-2-ynal I with O-silyl ketene O,S-acetal II (Bn = benzyl, TMS = trimethylsilyl) provided the syn-aldol product III, which was subsequently converted to (+)-bengamide E IV through optical resolution and the second diastereoselective aldol reaction as crucial steps.

IT 160840-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of begamide E via stereoselective aldol reaction of cobalt-complexed 4-methylpent-2-ynal with O-silyl ketene O,S-acetal)

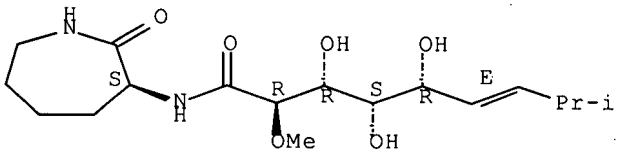
RN 160840-67-5 CAPLUS
CN D-gulo-Non-6-ynonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-4-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



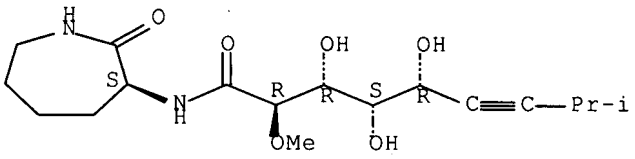
IT 118477-03-5P 160840-68-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of begamide E via stereoselective aldol reaction of cobalt-complexed 4-methylpent-2-ynal with O-silyl ketene O,S-acetal)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



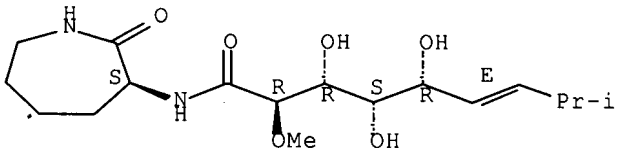
RN 160840-68-6 CAPLUS
CN D-gulo-Non-6-ynonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

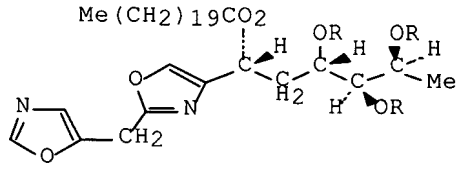


L10 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:579365 CAPLUS Full-text
DN 121:179365
TI Synthetic studies of some marine natural products from D-glucose
AU Kishimoto, Hisakazu; Ohrui, Hiroshi; Meguro, Hiroshi
CS Fac. Agric., Tohoku Univ., Sendai, 981, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1993), 35th, 112-19
CODEN: TYKYDS
DT Journal
LA Japanese
AB A report from a symposium describing the total synthesis of bengamide E from D-glucose and synthetic study of ciguatoxin.
IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthetic studies of some marine natural products from D-glucose)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:575545 CAPLUS Full-text
DN 121:175545
TI Amino acid derivatives from the marine sponge Jaspis digonoxea
AU Rudi, Amira; Kashman, Yoel; Benayahu, Yehuda; Schleyer, Michael
CS Sch. Chem., Tel Aviv Univ., Tel Aviv, 69978, Israel
SO Journal of Natural Products (1994), 57(6), 829-36
CODEN: JNPRDF; ISSN: 0163-3864
DT Journal
LA English
GI

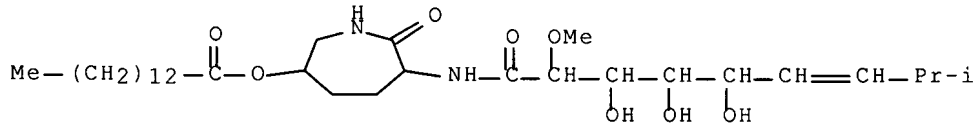


I, R=H
II, R=Ac

AB Six heterocycles, bengamide A, bengamide B, cyclo(L-trans-(4-hydroxyprolinyl)-L-phenylalanine), a functionalized nonene lactone, the novel digonazole (I), and cyclo(L-prolinyl-L-tyrosine), previously unreported from marine origin, were isolated from the South African sponge J. digonoxea. The structures of the known compds. and the new digonazole were elucidated primarily by NMR spectroscopy.

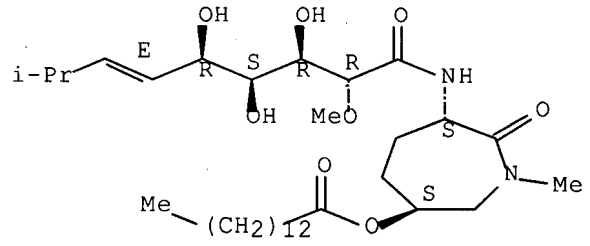
IT 104947-68-4, Bengamide A 104947-69-5, Bengamide B
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of marine sponge)

RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

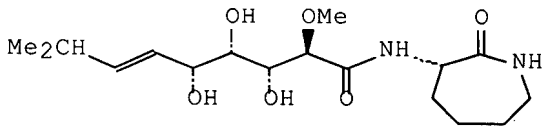


RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

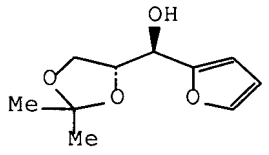
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



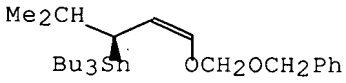
L10 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:31190 CAPLUS Full-text
DN 120:31190
TI Stereoselective total synthesis of bengamide E from glyceraldehyde acetonide and a nonracemic γ-alkoxy allylic stannane
AU Marshall, James A.; Luke, George P.
CS Dep. Chem. Biochem., Univ. South Carolina, Columbia, SC, 29208, USA
SO Journal of Organic Chemistry (1993), 58(23), 6229-34
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 120:31190
GI



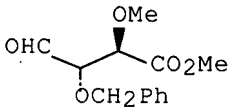
I



II



III



IV

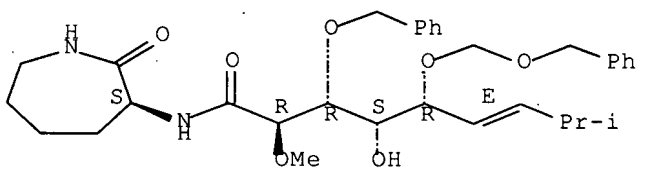
AB The synthesis of bengamide E (I) was achieved starting from the furan adduct II of (R)-glyceraldehyde acetonide. The key step entailed MgBr2-promoted addition of the (S)-γ-alkoxy allylic stannane III to the aldehyde IV obtained from the oxidation product of furan II after protection as the Me ether. The adduct of stannane III and aldehyde IV, a 1:1 hydroxy ester and lactone mixture, was converted to bengamide E by aminolysis with (S)-2-aminocaprolactam and subsequent debenzylation with Li in NH3.

IT 151867-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reductive deblocking of, bengamide E from)

RN 151867-47-9 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-5-O-[(phenylmethoxy)methyl]-3-O-(phenylmethyl)-, [1(S),6E]- (9CI) (CA INDEX NAME)

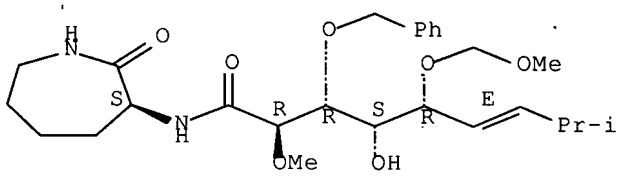
Absolute stereochemistry.
Double bond geometry as shown.



IT 146384-02-3P
RL: SPN (Synthetic preparation); PREP (Preparation)

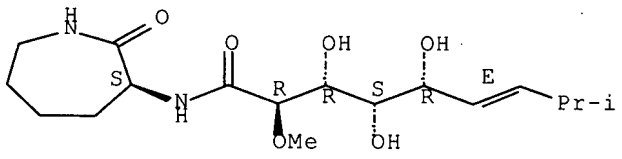
(preparation of)
RN 146384-02-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-5-O-(methoxymethyl)-8-methyl-2-O-methyl-3-O-(phenylmethyl)-, [1(S),6E]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

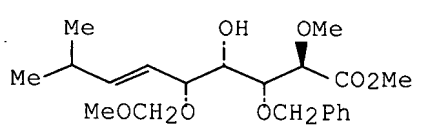


IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of, via addition of chiral (alkoxyallyl)stannane
to benzyloxy(methoxy)oxobutanoate)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

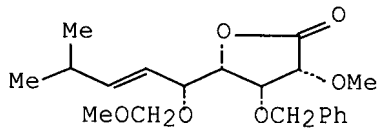
Absolute stereochemistry.
Double bond geometry as shown.



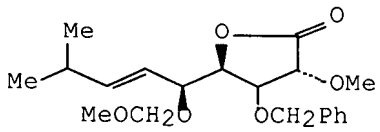
L10 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1993:147391 CAPLUS Full-text
DN 118:147391
TI Stereoselective synthesis of a bengamide E derivative through SE' addition of a chiral γ-alkoxy allylic stannane to a tartrate-derived α,β-dialkoxy aldehyde
AU Marshall, James A.; Luke, George P.
CS Dep. Chem. Biochem., Univ. South Carolina, Columbia, SC, 29208, USA
SO Synlett (1992), (12), 1007-8
CODEN: SYNLES; ISSN: 0936-5214
DT Journal
LA English
GI



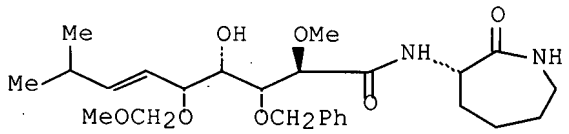
I



II



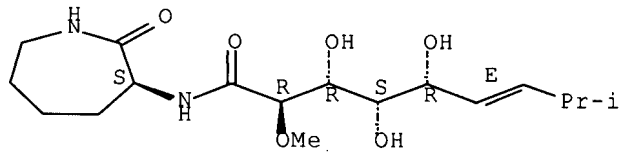
III



IV

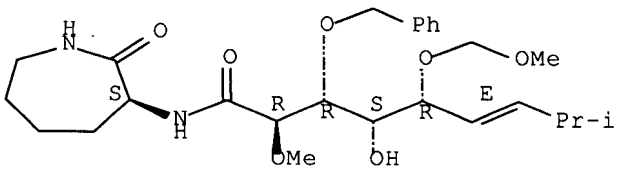
AB Addition of the (±)-(E)-Me2CH(SnBu3)CH:CHOCH2OMe, in three-fold excess, to the(S,R)-OCHCH(OCH2Ph)CH(OMe)CO2Me in the presence of MgBr2 afforded ester I and lactones II and III as a separable 1.2:1.4:1 mixture in 90% yield. The mixture of I and II was converted to the bengamide E precursor IV upon treatment with (S)-α-aminocaprolactam and Me3Al.
IT 118477-03-5DP, Bengamide E, ether protected
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 146384-02-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of, as bengamide E intermediate)
RN 146384-02-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-5-O-(methoxymethyl)-8-methyl-2-O-methyl-3-O-(phenylmethyl)-, [1(S),6E]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.


H
N
O
S
N
H
O
R
OMe
O
Ph
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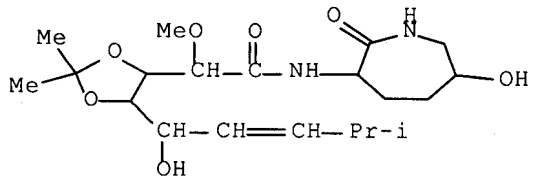
O
S
OH
O
OMe
R
E
Pr-i

L10 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:612932 CAPLUS Full-text
DN 117:212932
TI Total synthesis and absolute configuration of bengamide A
AU Chida, Noritaka; Tobe, Takahiko; Okada, Shinsuke; Ogawa, Seiichiro
CS Fac. Sci. Technol., Keio Univ., Yokohama, 223, Japan
SO Journal of the Chemical Society, Chemical Communications (1992), (15), 1064-6
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 117:212932
GI

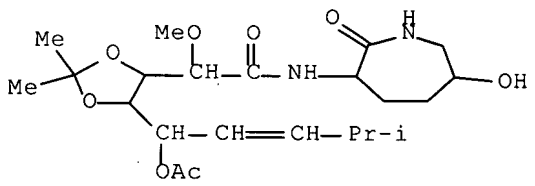
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The first total synthesis of the novel marine natural product, bengamide A (I) is described, revealing the absolute configuration of this compound I was prepared in several steps from known ester II (Boc = Me3O2C), which can be obtained from L-glutamic acid in 4 steps. Key steps were the cyclization of active ester III to give hexahydro-2-azepinone IV (R1 = CH2Ph, R2 = Boc) and the coupling of IV.CF3CO2H (R1 = R2 = H) with polyhydroxylated C10 side chain V by (EtO)2P(O)CN to give the corresponding amide.

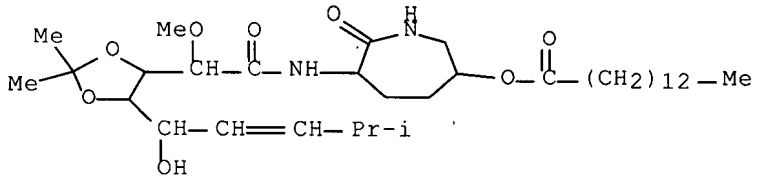
IT 144090-68-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of, with myristic acid)
RN 144090-68-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, [3S-[3α(E),6β]]- (9CI) (CA INDEX NAME)



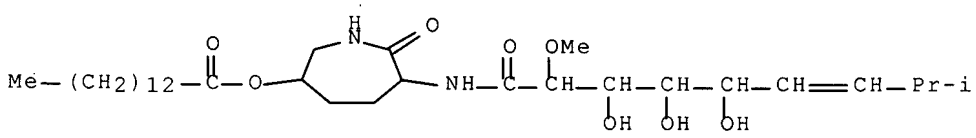
IT 144090-67-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
RN 144090-67-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, 5-acetate, [3S-[3α(E),6β]]- (9CI) (CA INDEX NAME)



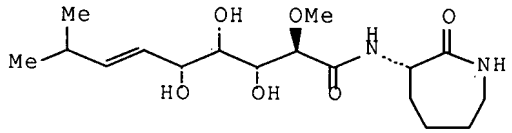
IT 144090-69-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 144090-69-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, [3S-[3α(E),6β]]- (9CI) (CA INDEX NAME)



IT 104947-68-4P, Bengamide A
RL: PRP (Properties); PREP (Preparation)
(total synthesis and absolute configuration of)
RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



L10 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:571976 CAPLUS Full-text
DN 117:171976
TI An enantioselective synthesis of bengamide E
AU Kishimoto, Hisakazu; Ohrui, Hiroshi; Meguro, Hiroshi
CS Fac. Agric., Tohoku Univ., Sendai, 981, Japan
SO Journal of Organic Chemistry (1992), 57(18), 5042-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 117:171976
GI

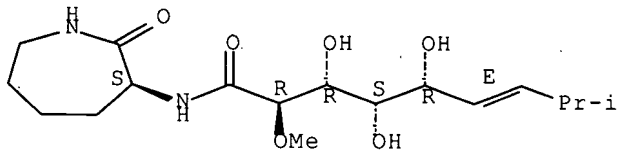


I

AB The total synthesis of bengamide E (I), a novel sponge-derived cyclolysine derivative, has been accomplished. The C10 side chain common to members of the bengamide family was prepared from D-glucose.

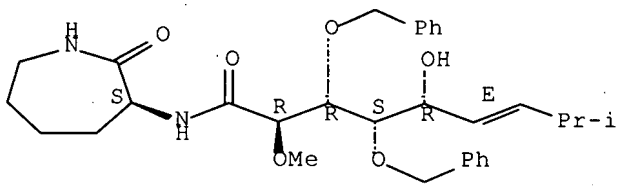
IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



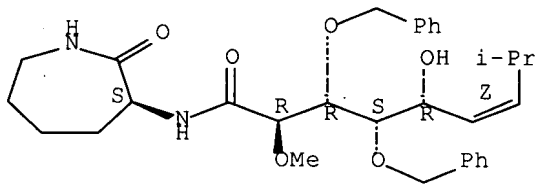
IT 142946-29-0P 142946-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 142946-29-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-3,4-bis-O-(phenylmethyl)-, [1(S),6E]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



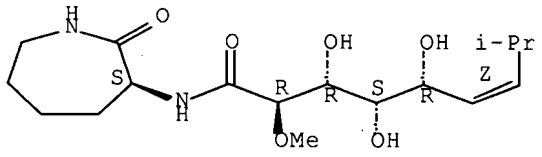
RN 142946-34-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-3,4-bis-O-(phenylmethyl)-, [1(S),6Z]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



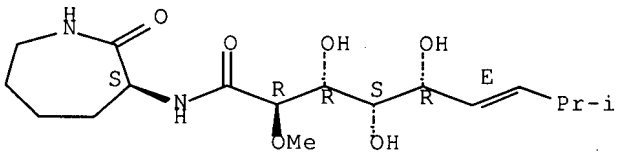
IT 143005-13-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 143005-13-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-, [1(S),6Z]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

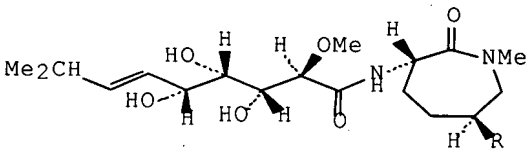


L10 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:152221 CAPLUS Full-text
DN 116:152221
TI Syntheses of natural products starting from cyclitols
AU Chida, N.; Tobe, T.; Furuno, Y.; Ogawa, S.
CS Fac. Sci. Technol., Keio Univ., Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1991), 33rd, 275-82
CODEN: TYKYDS
DT Journal
LA Japanese
AB A symposium on the total synthesis of (+)- and (-)-nojirimycin from myo-inositol, (-)-isoavenaciolide and (-)-ethisolide from L-quebrachitol, and bengamide E from L-quebrachitol.
IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from quebrachitol)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:6937 CAPLUS Full-text
DN 116:6937
TI Enantioselective total syntheses of bengamides B and E
AU Broka, Chris A.; Ehrler, Jurg
CS Inst. Bio-Org. Chem., Syntex Res., Palo Alto, CA, 94304, USA
SO Tetrahedron Letters (1991), 32(42), 5907-10
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 116:6937
GI

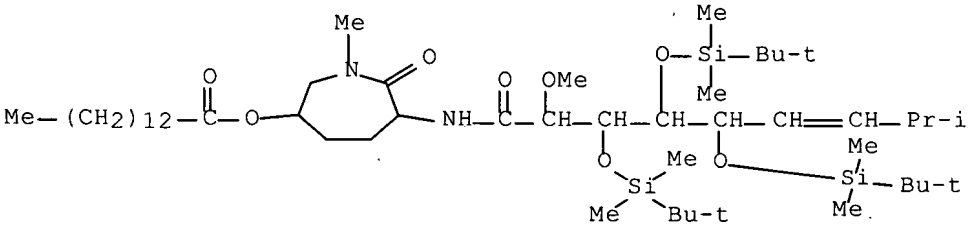


I

AB Convergent total syntheses of two sponge-derived cyclolysine derivs., bengamides B [I; R = Me(CH2)12CO2] (II) and E (I; R = H) have been accomplished. The polyhydroxylated side chain common to both natural products was obtained from L-glucose and the hydroxylated caprolactam moiety of II was prepared using oxazolidinone chemical of D. A. Evans, et. al. (1987, 1988). In the course of this work, a new Horner-Emmons reagent incorporating one of the chiral auxiliaries of D. A. Evans was developed.

IT 137789-58-3P 137789-59-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of)

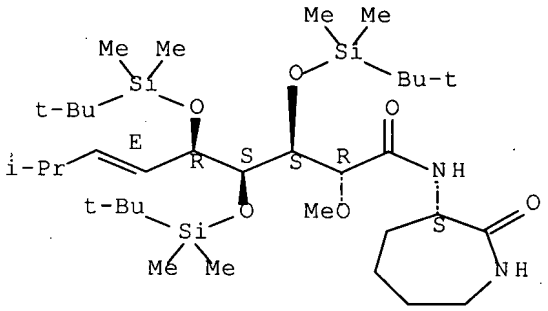
RN 137789-58-3 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-3,4,5-tris-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, [1(3S,6S),6E]-(9CI) (CA INDEX NAME)



RN 137789-59-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-3,4,5-tris-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-

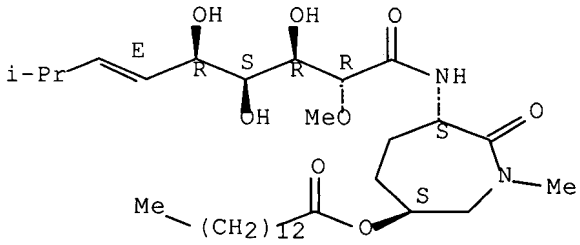
methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



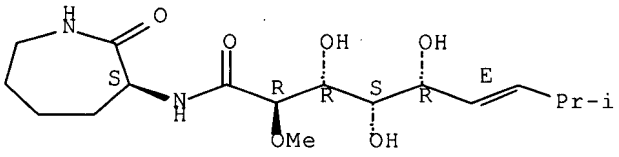
IT 104947-69-5P, Bengamide B 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

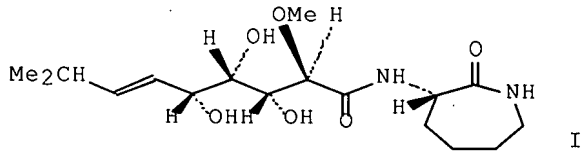


RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



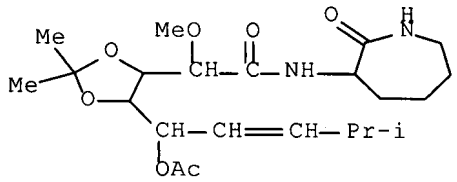
L10 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1991:472162 CAPLUS Full-text
DN 115:72162
TI Total synthesis of bengamide E
AU Chida, Noritaka; Tobe, Takahiko; Ogawa, Seiichiro
CS Fac. Sci. Technol., Keio Univ., Yokohama, 223, Japan
SO Tetrahedron Letters (1991), 32(8), 1063-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 115:72162
GI



I

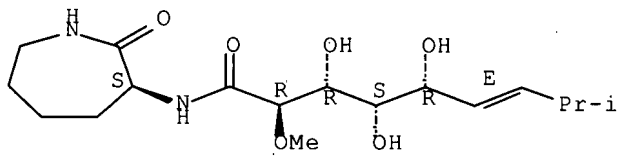
AB The 1st total synthesis of bengamide E (I), a novel sponge-derived amino acid, is described. The side chain of bengamide E, possessing 4 contiguous chiral centers, was prepared in a stereoselective manner starting from naturally abundant cyclitol, L-quebrachitol.

IT 134936-16-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
RN 134936-16-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-3,4-O-(1-methylethylidene)-, 5-acetate, (6E)- (9CI) (CA INDEX NAME)

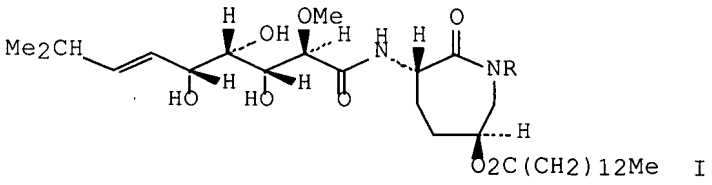


IT 118477-03-5P, Bengamide E
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of, from quebrachitol)
RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

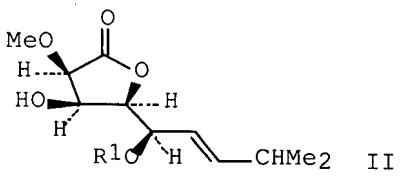
Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1990:36408 CAPLUS Full-text
DN 112:36408
TI Novel sponge-derived amino acids. 11. The entire absolute stereochemistry of the bengamides
AU Adamczeski, Madeline; Quinoa, Emilio; Crews, Phillip
CS Dep. Chem., Univ. California, Santa Cruz, CA, 95064, USA
SO Journal of Organic Chemistry (1990), 55(1), 240-2
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 112:36408
GI



I



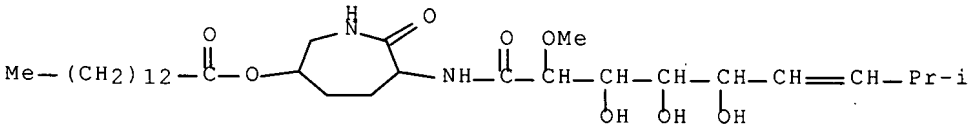
II

AB The complete stereochem. of bengamides A and B (I, R = H, Me) can be assigned as 5R,6S,7R,8R,10S,13S, and this absolute stereochem. can also be extended to other bengamide derivs. C, D, E, F, and isobengamide E. The absolute stereochem. results were obtained by isolating monohydroxy lactone II [R1 = Me(CH2)12CO] (III) which was then converted to dihydroxy lactone II (R1 = H). The relative stereochem. of II (R1 = H) had been previously shown to be the same as that of the 2-methoxy-3,4,5-trihydroxy-8-methylnon- 6(E)-enoyl side chain in the bengamides. The absolute stereochem. of lactone III, deduced by esterifying with O-methylmandelic acids followed by an anal. of their different 1H NMR chemical shifts, gave the absolute configuration of the stereocenters in the side chain. Combining the new assignments with those obtained previously for the δ-hydroxycaprolactam moiety of the bengamides completed assignment of the absolute configuration at all chiral sites.

IT 104947-68-4, Bengamide A 104947-69-5, Bengamide B
104975-72-6, Bengamide C 118477-02-4, Bengamide D
118477-03-5, Bengamide E 118477-04-6, Bengamide F
RL: PRP (Properties)
(absolute configuration of)

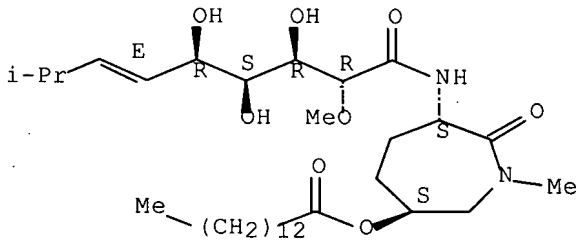
RN 104947-68-4 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



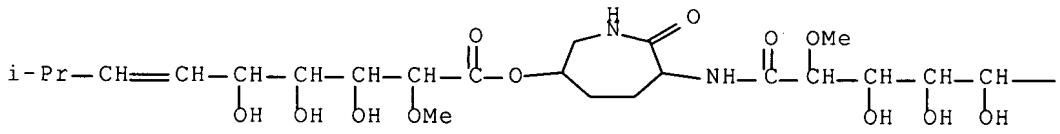
RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

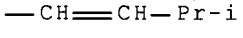


RN 104975-72-6 CAPLUS
CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A

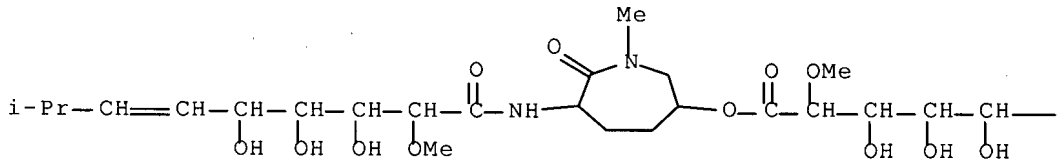


PAGE 1-B

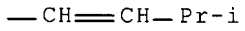


RN 118477-02-4 CAPLUS
CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-1-methyl-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A

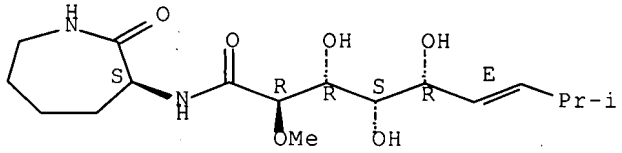


PAGE 1-B

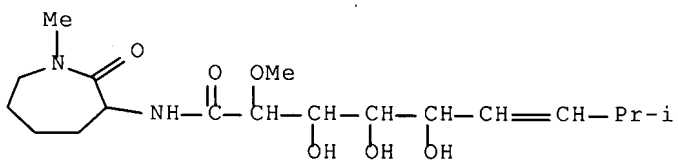


RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



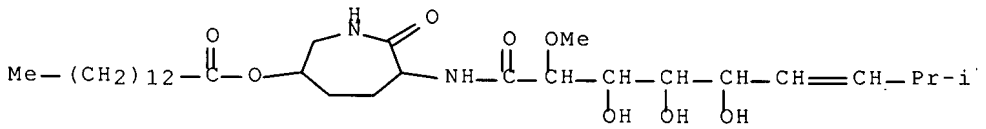
RN 118477-04-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



L10 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:520942 CAPLUS Full-text
DN 111:120942
TI Bengamide anthelmintics
IN Crews, Philip; Matthews, Thomas R.; Quinoa, Emilio; Adamczeski, Madeline
PA University of California, Berkeley, USA; Syntex (U.S.A.), Inc.
SO U.S., 8 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

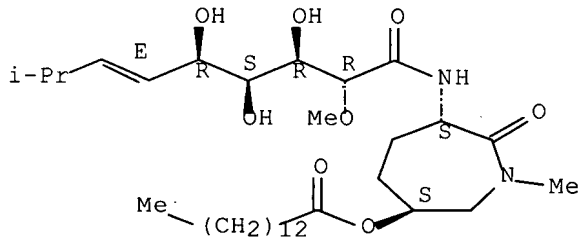
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4831135	A	19890516	US 1986-875486	19860618
PRAI	US 1986-875486		19860618		

OS MARPAT 111:120942
GI For diagram(s), see printed CA Issue.
AB δ-Caprolactam derivs. (I; R = H, lower alkyl, lower alkanoyl; R1-R3, R5 = H, lower alkanoyl; R4 = H, C1-22-alkanoyl; R6, R7 = H, OH; R6R7 = epoxide or double bond) and their salts are anthelmintics (no data). I (R-R3, R5 = H; R4 = tetradecanoyl; R6R7 = double bond) (bengamide A) and I (R = Me, R1-R3, R5 = H; R4 = tetradecanoyl; R6R7 = double bond) (bengamide B) was extracted from Jaspidae sponge using MeOH. A tablet formulation contained bengamide I (R = H, Me; R1-R3, R5 = H; R4 = tetradecanoyl; R6R7 = double bond) 5.0, Mg stearate 0.75, starch 0.75, lactose 29.0, and PVP 0.75 parts.
IT 104947-68-4 104947-69-5, Bengamide B
RL: BIOL (Biological study)
(anthelmintic)
RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



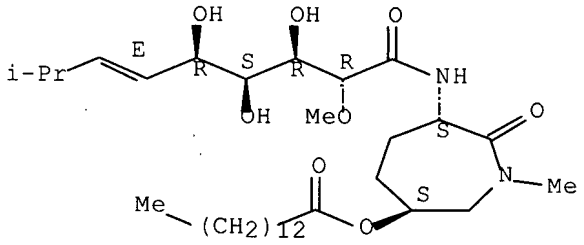
IT 122467-31-6
RL: BIOL (Biological study)
(anthelmintic pharmaceuticals containing)
RN 122467-31-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-,

[1(3S,6S),6E]-, mixt. with [1(3S,6S),6E]-6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-D-gulo-non-6-enonamide (9CI) (CA INDEX NAME)

CM 1

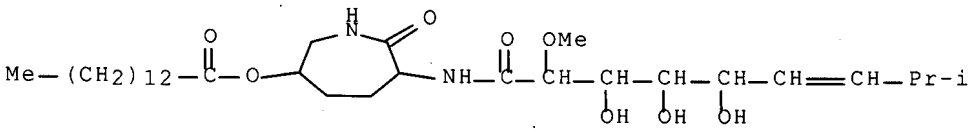
CRN 104947-69-5
CMF C32 H58 N2 O8

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

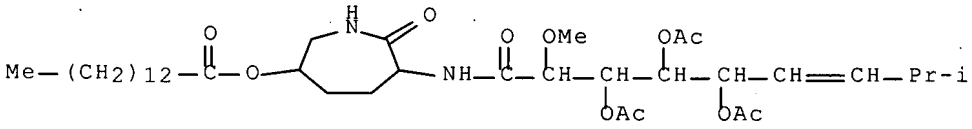


CM 2

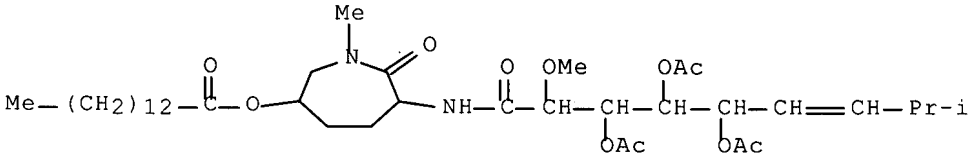
CRN 104947-68-4
CMF C31 H56 N2 O8



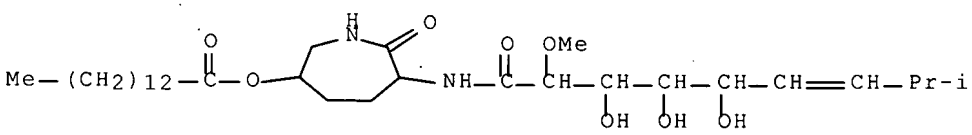
IT 104975-81-7P 104975-82-8P
RL: THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)(preparation of, as anthelmintic)
RN 104975-81-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)



RN 104975-82-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)

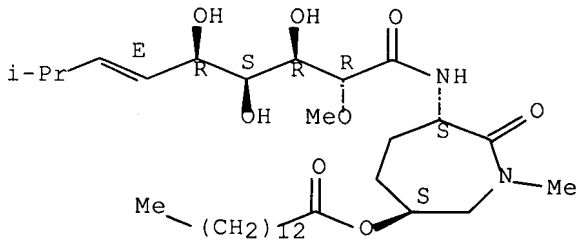


L10 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:72745 CAPLUS Full-text
DN 110:72745
TI Novel sponge-derived amino acids. 5. Structures, stereochemistry, and synthesis of several new heterocycles
AU Adamczeski, Madeline; Quinoa, Emilio; Crews, Phillip
CS Dep. Chem., Univ. California, Santa Cruz, CA, 95064, USA
SO Journal of the American Chemical Society (1989), 111(2), 647-54
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB The complete amino acid chemical of an undescribed Jaspidae sponge, collected annually in the Benga lagoon of the Fiji Islands during 1984-1987 is described. Five different amino acid types are represented among its constituents and include the bengamides (6 compds.), isobengamide E, bengazoles (A and B), a dioxopiperazine cyclo(L-trans-(4-hydroxy-Pro-L- Phe), and N-acetyl-L-phenylalanine Me ester. The structures and stereochem. features of the bengamides were established by relying on analogies to bengamides A and B, along with insights gained by extensive spectroscopic and chemical degradation of isobengamide E and bengamide E. The chirality of the substituted ε-caprolactam ring of the bengamides was established as 10S and 13S by a combination of mol. mechanics calcns. and hydrolysis of isobengamide E and bengamide E fragmentation products to obtain L-lysine HCl. The relative stereochem. of the 2(R*)-methoxy- 3(R*),4(S*),5(R*)-trihydroxy-8-methylnonan-6(E)-enoyl side chain of the bengamides was based on anal. of 1H NMR J values of cyclized products. The bengazole structures have been previously established, and the structures of the remaining 2 amino acids were verified by synthesis. Biogenetic pathways are suggested for each of the most novel amino acid types.
IT 104947-68-4, Bengamide A 104947-69-5, Bengamide B
104975-72-6, Bengamide C 118477-02-4 118477-03-5
118477-04-6 118477-11-5 118477-12-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, isolation and mol. structure of)
RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

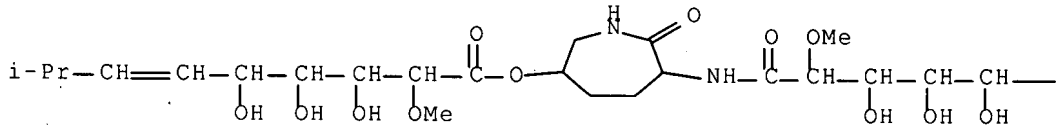
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



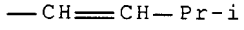
RN 104975-72-6 CAPLUS

CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



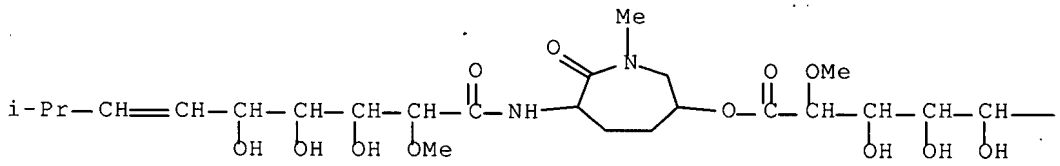
PAGE 1-B



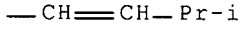
RN 118477-02-4 CAPLUS

CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-1-methyl-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A

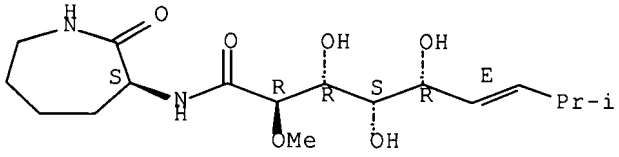


PAGE 1-B

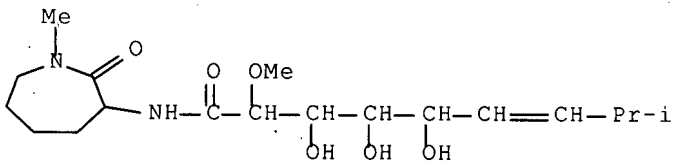


RN 118477-03-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

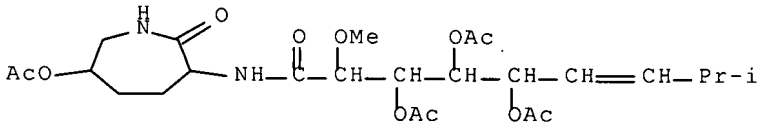
Absolute stereochemistry.
Double bond geometry as shown.



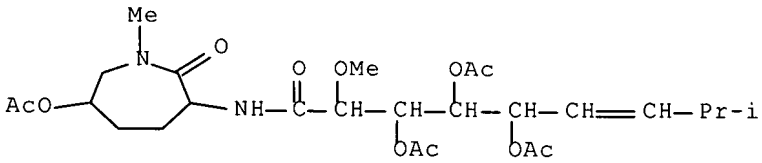
RN 118477-04-6 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S)-hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)



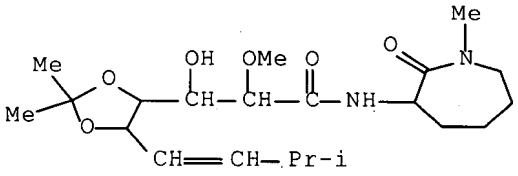
RN 118477-11-5 CAPLUS
CN D-gulo-Non-6-enonamide, N-[6-(acetyloxy)hexahydro-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, 3,4,5-triacetate, [3S-[3α(E),6β]]- (9CI) (CA INDEX NAME)



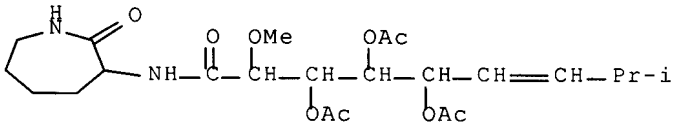
RN 118477-12-6 CAPLUS
CN D-gulo-Non-6-enonamide, N-[6-(acetyloxy)hexahydro-1-methyl-2-oxo-1H-azepin-3-yl]-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, 3,4,5-triacetate, [3S-[3α(E),6β]]- (9CI) (CA INDEX NAME)



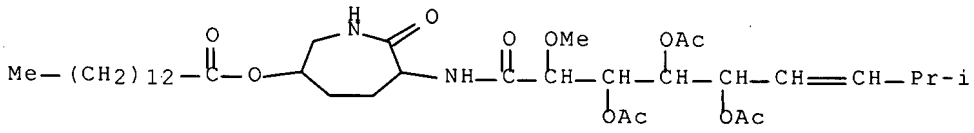
IT 118477-17-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
RN 118477-17-1 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-1-methyl-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-4,5-O-(1-methylethylidene)-, [1(S),6E]- (9CI) (CA INDEX NAME)



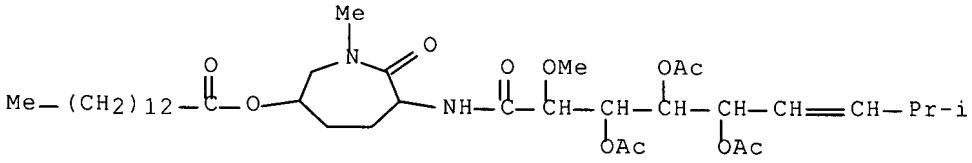
IT 118477-15-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and basic hydrolysis and acetylation of)
RN 118477-15-9 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(S),6E]- (9CI) (CA INDEX NAME)



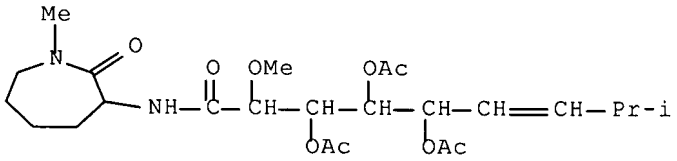
IT 104975-81-7P 104975-82-8P 118477-16-0P
118494-65-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 104975-81-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)



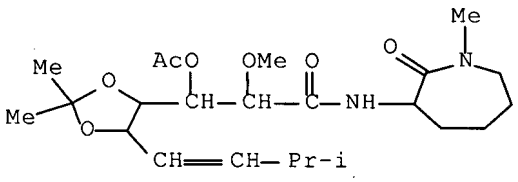
RN 104975-82-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)



RN 118477-16-0 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-1-methyl-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(S),6E]- (9CI) (CA INDEX NAME)

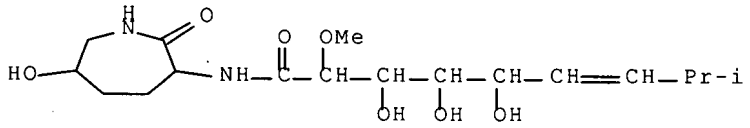


RN 118494-65-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-(hexahydro-1-methyl-2-oxo-1H-azepin-3-yl)-8-methyl-2-O-methyl-4,5-O-(1-methylethylidene)-, 3-acetate, [1(S),6E]- (9CI) (CA INDEX NAME)



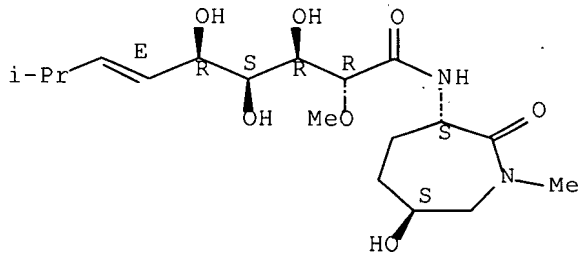
IT 118477-09-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by acid-catalyzed fragmentation of bengamide C)
RN 118477-09-1 CAPLUS

CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

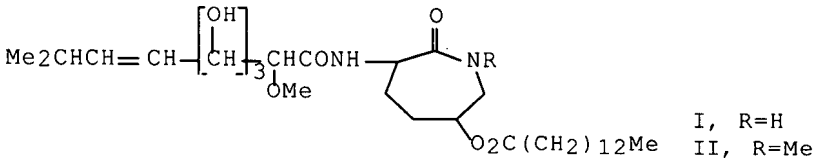


IT 118477-10-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by acid-catalyzed fragmentation of bengamide D)
RN 118477-10-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-6-hydroxy-1-methyl-2-oxo-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



L10 ANSWER 53 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1987:15950 CAPLUS Full-text
DN 106:15950
TI Bengamides, heterocyclic anthelmintics from a Jaspidae marine sponge
AU Quinoa, Emilio; Adamczeski, Madeline; Crews, Phillip; Bakus, Gerald J.
CS Inst. Mar. Stud., Univ. California, Santa Cruz, CA, 95064, USA
SO Journal of Organic Chemistry (1986), 51(23), 4494-7
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
GI



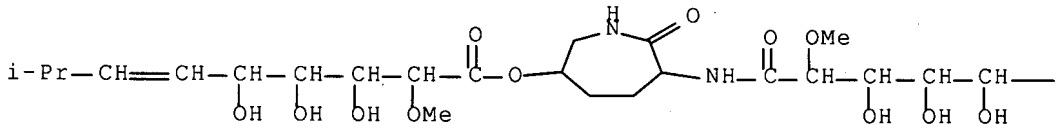
I, R=H
II, R=Me

AB The MeOH extract of an undescribed Fiji sponge of the Jaspidae family contained the novel 7-membered ring heterocyclic compds. bengamide A (I) and bengamide B (II). A 3rd compound, bengamide C, was also isolated but was not purified completely. The structure of I and II were determined by spectroscopy, primarily 13C-NMR, and by chemical degradation anal. All 3 compds. were biotoxic to eukaryotic cells, nematodes, and bacteria. I and II were completely toxic to Nippostrongylus braziliensis at 50μg/mL.

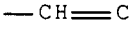
IT 104975-72-6
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, antihelmintic activity of)

RN 104975-72-6 CAPLUS
CN D-gulo-Non-6-enonic acid, 6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-, (3S,6S)-hexahydro-7-oxo-6-[[(6E)-6,7,8,9-tetradeoxy-8-methyl-2-O-methyl-D-gulo-non-6-enonoyl]amino]-1H-azepin-3-yl ester, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A

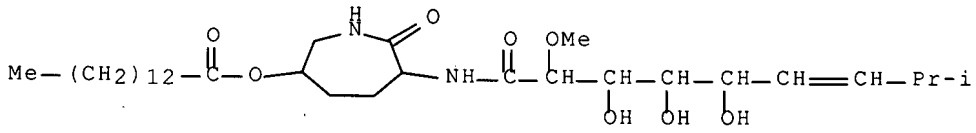


PAGE 1-B



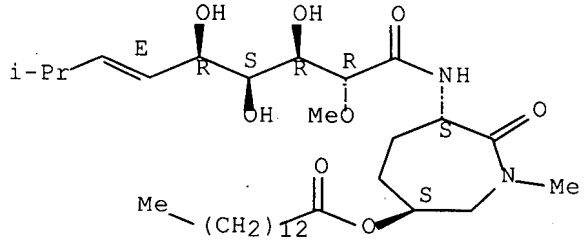
IT 104947-68-4 104947-69-5
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge, isolation and mol. structure and antihelmintic activity of)

RN 104947-68-4 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)- (9CI) (CA INDEX NAME)

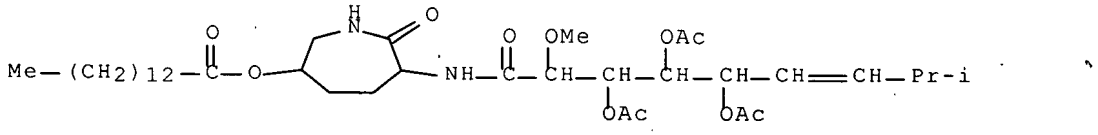


RN 104947-69-5 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, (6E)-(9CI) (CA INDEX NAME)

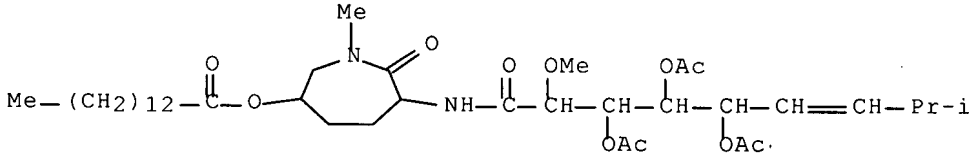
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT 104975-81-7P 104975-82-8P
RL: SPN (Synthetic preparation); PREP (Preparation)(preparation of)
RN 104975-81-7 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)



RN 104975-82-8 CAPLUS
CN D-gulo-Non-6-enonamide, 6,7,8,9-tetradeoxy-N-[hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1H-azepin-3-yl]-8-methyl-2-O-methyl-, 3,4,5-triacetate, [1(3S,6S),6E]- (9CI) (CA INDEX NAME)



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=> d l2; d l7; d his; log y
L2 HAS NO ANSWERS
L1              STR
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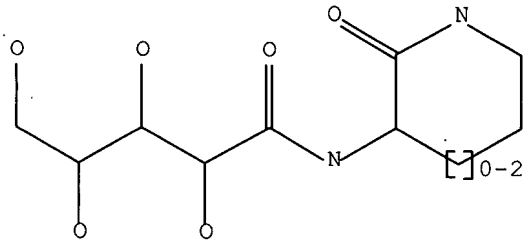


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Structure attributes must be viewed using STN Express query preparation.
L2              QUE  ABB=ON  PLU=ON  L1

L7 HAS NO ANSWERS
L6              STR
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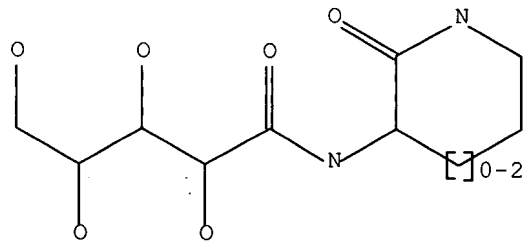


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Structure attributes must be viewed using STN Express query preparation.
L7              QUE  ABB=ON  PLU=ON  L6

     (FILE 'HOME' ENTERED AT 17:13:24 ON 10 JUN 2007)

     FILE 'REGISTRY' ENTERED AT 17:13:37 ON 10 JUN 2007
L1              STRUCTURE UPLOADED
L2              QUE L1
L3            4 S L2
L4          240 S L2 FUL

     FILE 'CAPLUS' ENTERED AT 17:14:49 ON 10 JUN 2007
L5           53 S L4

     FILE 'REGISTRY' ENTERED AT 17:15:53 ON 10 JUN 2007
L6              STRUCTURE UPLOADED
L7              QUE L6
L8            9 S L7 SAM SUB=L4
L9          236 S L7 FUL SUB=L4

     FILE 'CAPLUS' ENTERED AT 17:16:55 ON 10 JUN 2007
L10          53 S L9

COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             277.42     492.67

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                             -39.78     -39.78

STN INTERNATIONAL LOGOFF AT 17:18:53 ON 10 JUN 2007
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